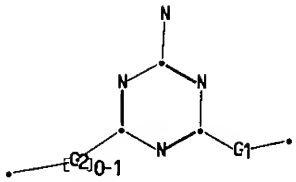
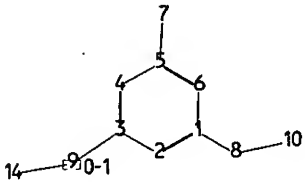
L Number	Hits	Search Text	DB	Time stamp
1	4285	HDL	USPAT; US-PGPUB; EPO; JPO; DERWENT	2002/05/19 10:49
2	1525	HDL adj cholester$	USPAT; US-PGPUB; EPO; JPO; DERWENT	2002/05/19 10:49
3	1912731	rais$ or elevat$	USPAT; US-PGPUB; EPO; JPO; DERWENT	2002/05/19 10:50
4	423	(HDL adj cholester$) same (rais$ or elevat$)	USPAT; US-PGPUB; EPO; JPO; DERWENT	2002/05/19 11:04
5	311	514/245.ccls.	USPAT; US-PGPUB; EPO; JPO; DERWENT	2002/05/19 11:05
6	0	544/213.ccls	USPAT; US-PGPUB; EPO; JPO; DERWENT	2002/05/19 11:06
7	176	544/213.ccls.	USPAT; US-PGPUB; EPO; JPO; DERWENT	2002/05/19 11:06
8	477	514/245.ccls. or 544/213.ccls.	USPAT; US-PGPUB; EPO; JPO; DERWENT	2002/05/19 11:06
9	0	((HDL adj cholester$) same (rais$ or elevat$)) and (514/245.ccls. or 544/213.ccls.)	USPAT; US-PGPUB; EPO; JPO; DERWENT	2002/05/19 11:07
10	52757	triazin$	USPAT; US-PGPUB; EPO; JPO; DERWENT	2002/05/19 11:07
11	28	((HDL adj cholester$) same (rais$ or elevat$)) and triazin$	USPAT; US-PGPUB; EPO; JPO; DERWENT	2002/05/19 11:07

C:\STNEXP4\QUERIES\10005064 (method).str





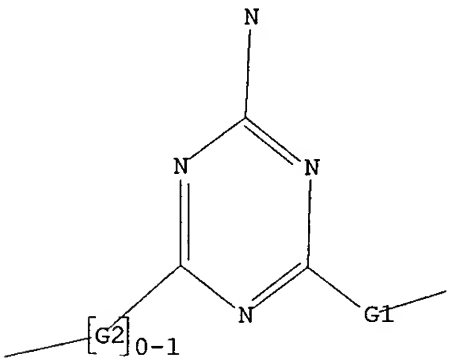
chain nodes :
8
ring nodes :
1 2 3 4 5 6
ring/chain nodes :
7 9 10 14
chain bonds :
1-8 3-9 5-7 8-10 9-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-8 3-9 5-7 8-10 9-14
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:O,S,N

G2:C,O

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
14:CLASS

```
=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 2016 OR  2026 OR  2039 OR  2040

L1    SCREEN CREATED

=>
Uploading C:\STNEXP4\QUERIES\10005064 (method).str

L2      STRUCTURE UPLOADED

=> que L2 NOT L1

L3   QUE L2 NOT L1

=> d l3
L3 HAS NO ANSWERS
L1               SCR 2016 OR 2026 OR 2039 OR 2040
L2               STR
```




```
G1 O,S,N
G2 C,O


Structure attributes must be viewed using STN Express query preparation.
L3               QUE  L2 NOT L1


=> s l3 sss sam
SAMPLE SEARCH INITIATED 11:44:16 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   3903 TO ITERATE

 25.6% PROCESSED    1000 ITERATIONS                          50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        74316 TO    81804
PROJECTED ANSWERS:           21441 TO    25551
```

```
L4            50 SEA SSS SAM L2 NOT L1

=> s l3 sss ful
FULL SEARCH INITIATED 11:44:23 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  76867 TO ITERATE

100.0% PROCESSED   76867 ITERATIONS                          23143 ANSWERS
SEARCH TIME: 00.00.04

L5         23143 SEA SSS FUL L2 NOT L1

=> s l5
L6          6375 L5

=> s hdl cholester?
          15172 HDL
         140259 CHOLESTER?
L7         6515 HDL CHOLESTER?
                  (HDL(W)CHOLESTER?)

=> s l6 (l) l7
L8             0 L6 (L) L7

=> s l6(l)l7
L9             0 L6(L)L7

=> s l6(p)l7
L10            0 L6(P)L7

=> s l6 and l7
L11            0 L6 AND L7

=> s cholester?
L12       140259 CHOLESTER?

=> s l6 (l) l12
L13            1 L6 (L) L12

=> d l13 bib,ab,hitstr
```

```
=> s abca? (w) express?
          306 ABCA?
       844177 EXPRESS?
L14         25 ABCA? (W) EXPRESS?

=> s abca? (p) express?
          306 ABCA?
       844177 EXPRESS?
L15         95 ABCA? (P) EXPRESS?

=> s l6 and l15
L16          0 L6 AND L15

=> d his

     (FILE 'HOME' ENTERED AT 11:42:59 ON 19 MAY 2002)

     FILE 'REGISTRY' ENTERED AT 11:43:04 ON 19 MAY 2002
L1                SCREEN 2016 OR  2026 OR  2039 OR  2040
L2                STRUCTURE UPLOADED
L3                QUE L2 NOT L1
L4             50 S L3 SSS SAM
L5          23143 S L3 SSS FUL

     FILE 'CAPLUS' ENTERED AT 11:44:33 ON 19 MAY 2002
L6          6375 S L5
L7          6515 S HDL CHOLESTER?
L8             0 S L6 (L) L7
L9             0 S L6(L)L7
L10            0 S L6(P)L7
L11            0 S L6 AND L7
L12       140259 S CHOLESTER?
L13            1 S L6 (L) L12
L14           25 S ABCA? (W) EXPRESS?
L15           95 S ABCA? (P) EXPRESS?
L16            0 S L6 AND L15

=> s coronary arter? or atheroscler?
          44483 CORONARY
         161715 ARTER?
          20291 CORONARY ARTER?
                  (CORONARY(W)ARTER?)
          32911 ATHEROSCLER?
L17       50483 CORONARY ARTER? OR ATHEROSCLER?

=> s l6 and l17
L18          3 L6 AND L17

=> d l18 1-3 bib,ab,hitstr
```

L18 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2002 ACS
AN 2002:90040 CAPLUS
DN 136:135022
TI Preparation of heteroaryl-.beta.-alanine derivatives as antiinflammatory agents and .alpha.4 integrin inhibitors
IN Konradi, Andrei W.; Pleiss, Michael A.; Thorsett, Eugene D.; Ashwell, Susan; Welmaker, Gregory S.; Kreft, Anthony; Sarantakis, Dimitrios; Dressen, Darren B.; Grant, Francine S.; Semko, Christopher; Xu, Ying-Zi
PA Elan Pharmaceuticals, Inc., USA; American Home Products Corporation
SO PCT Int. Appl., 141 pp.
CODEN: PIXXD2
DT Patent
LA English

not prior art

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002008222	A2	20020131	WO 2001-US23096	20010720

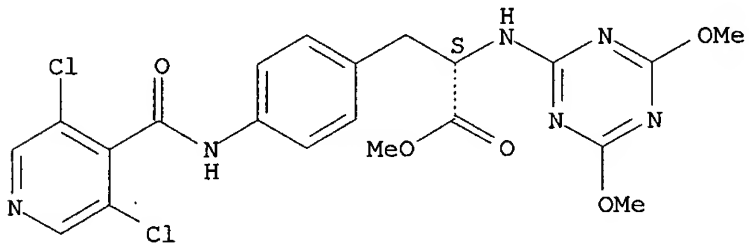
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI US 2000-220128P P 20000721
OS MARPAT 136:135022
AB Disclosed are a series of heteroaryl-.beta.-alanine derivs. I wherein R is a carboxylic acid; R1 and R2 are independently selected from the group consisting of hydrogen, alkyl, substituted alkyl, alkenyl, substituted alkenyl, cycloalkyl, substituted cycloalkyl, or R1 and R2, together with the nitrogen atom to which they are attached, are joined to form an optionally substituted heterocyclic ring provided that said substituted alkyl, substituted alkenyl and substituted cycloalkyl do not carry an aryl, substituted aryl, heteroaryl or substituted heteroaryl group; Ra and R3 are independently a hydrogen or a Me group; R4 and R5 are independently selected from the group consisting of heteroatom group; n is zero or an integer 1; Alk is a straight or branched alkylene chain; Ar is an optionally substituted arom. or heteroarom. group, as well as their pharmaceutical use as .alpha.4.beta.7 Integrin inhibitors for the treatment of inflammatory diseases. Thus, 3-[4-(3,5-dichloropyrid-4-ylcarboxamido)phenyl]-2-(3-chlorophenylamino)propanoic acid was prepd. as .alpha.4 Integrin inhibitor. The preferred compds. of the invention generally have IC50 values in the .alpha.4.beta.1 and .alpha.a.beta.7 assays of 1 .mu.M and below. In the other assays featuring .alpha. integrins of other subgroups the same compds. had IC50 values of 50 .mu.M and above thus demonstrating the potency and selectivity of their action against .alpha.4 integrins. Title compds. were prepd. for treating an inflammatory condition in a mammalian patient which condition is mediated by Very Late Antigen 4 (VLA-4). Inflammatory condition is selected from the group consisting of asthma, Alzheimer's disease, **atherosclerosis**, AIDS dementia, diabetes, inflammatory bowel disease, multiple sclerosis, rheumatoid arthritis, tissue transplantation, tumor metastasis, meningitis, encephalitis, stroke, nephritis, retinitis, atopic dermatitis, psoriasis, myocardial ischemia and acute leukocyte-mediated lung injury.
IT **263274-37-9P 263274-66-4P 263274-86-8P**

263274-93-7P 263274-94-8P 263274-95-9P
263274-97-1P 263274-99-3P 263275-01-0P
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of heteroaryl-.beta.-alanine derivs. as antiinflammatory agents and .alpha.4 integrin inhibitors)

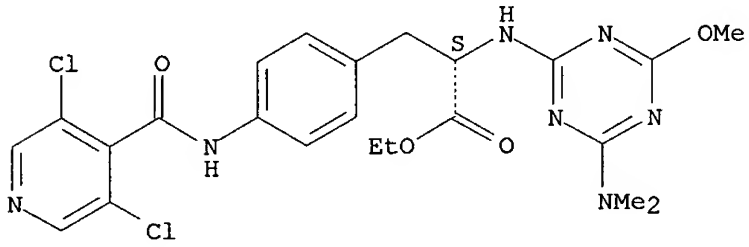
RN 263274-37-9 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



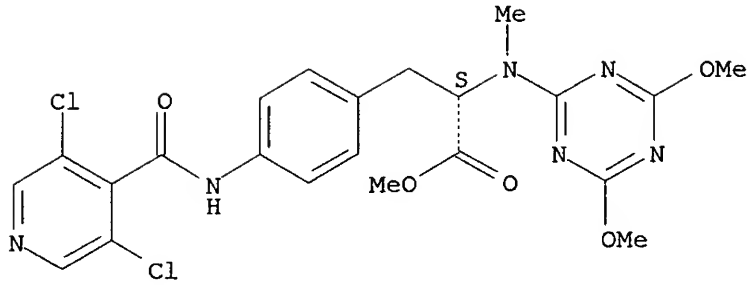
RN 263274-66-4 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[4-(dimethylamino)-6-methoxy-1,3,5-triazin-2-yl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



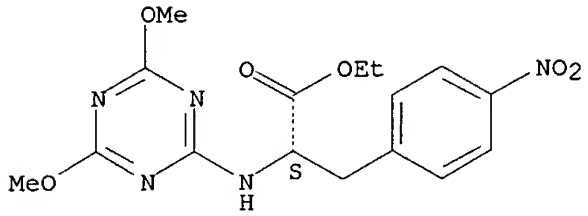
RN 263274-86-8 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-N-methyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



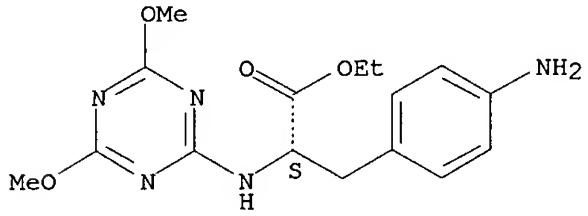
RN 263274-93-7 CAPLUS
CN L-Phenylalanine, N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-4-nitro-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



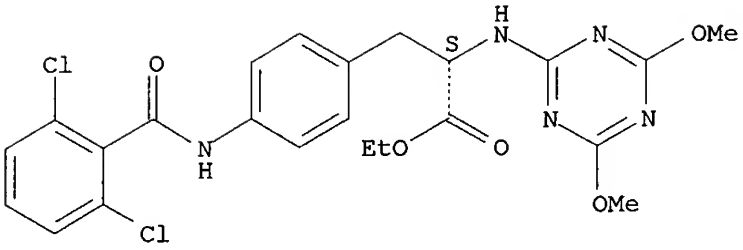
RN 263274-94-8 CAPLUS
CN L-Phenylalanine, 4-amino-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



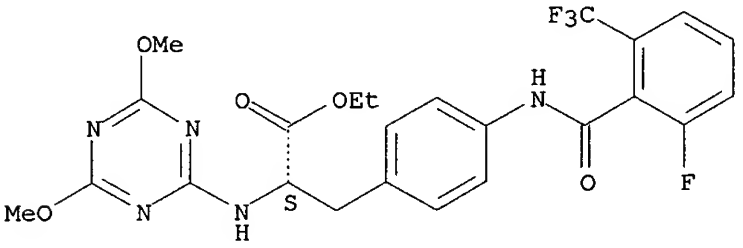
RN 263274-95-9 CAPLUS
CN L-Phenylalanine, 4-[(2,6-dichlorobenzoyl)amino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



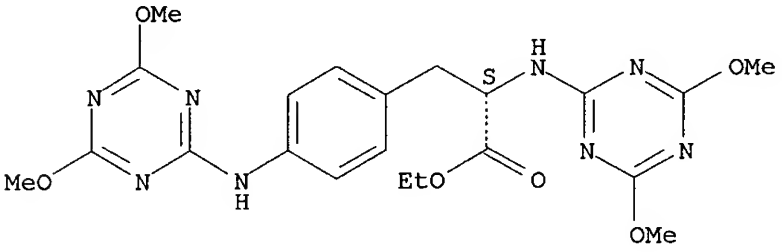
RN 263274-97-1 CAPLUS
CN L-Phenylalanine, N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-4-[[2-fluoro-6-(trifluoromethyl)benzoyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



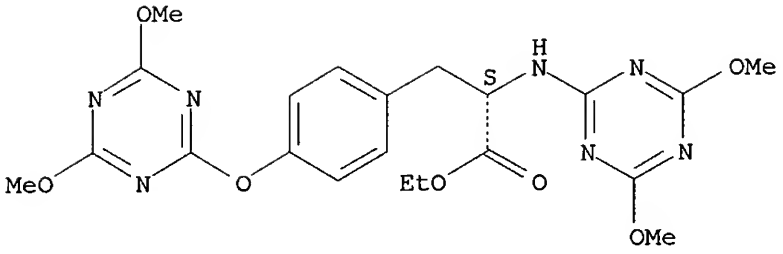
RN 263274-99-3 CAPLUS
CN L-Phenylalanine, N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-4-[(4,6-dimethoxy-1,3,5-triazin-2-yl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 263275-01-0 CAPLUS
CN L-Tyrosine, N,O-bis(4,6-dimethoxy-1,3,5-triazin-2-yl)-, ethyl ester (9CI) (CA INDEX NAME)

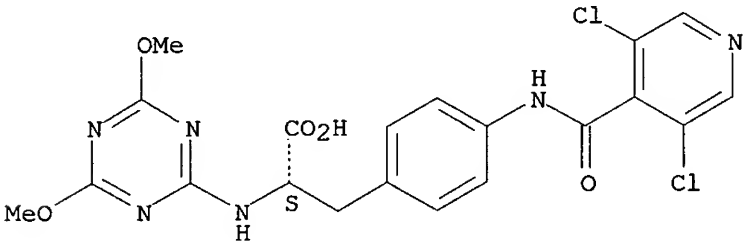
Absolute stereochemistry.



IT **263274-38-0P 263274-67-5P 263274-68-6P**
263274-69-7P 263274-70-0P 263274-71-1P
263274-72-2P 263274-73-3P 263274-74-4P
263274-75-5P 263274-76-6P 263274-85-7P
263274-87-9P 263274-88-0P 263274-89-1P
263274-90-4P 263274-96-0P 263274-98-2P
263275-00-9P 263275-02-1P 263275-03-2P
263275-04-3P
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of heteroaryl-.beta.-alanine derivs. as antiinflammatory agents and .alpha.4 integrin inhibitors)

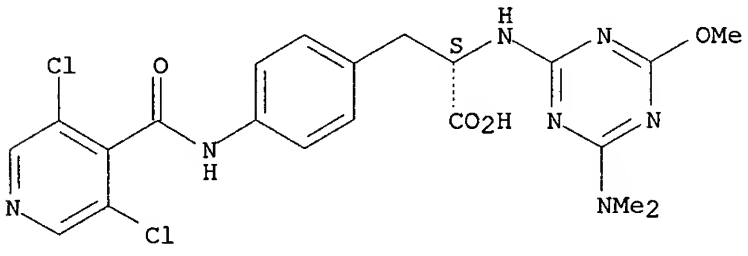
RN 263274-38-0 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



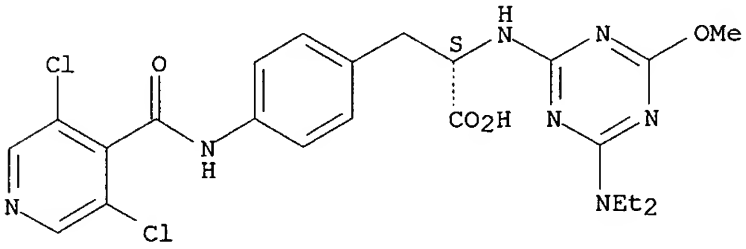
RN 263274-67-5 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[4-(dimethylamino)-6-methoxy-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



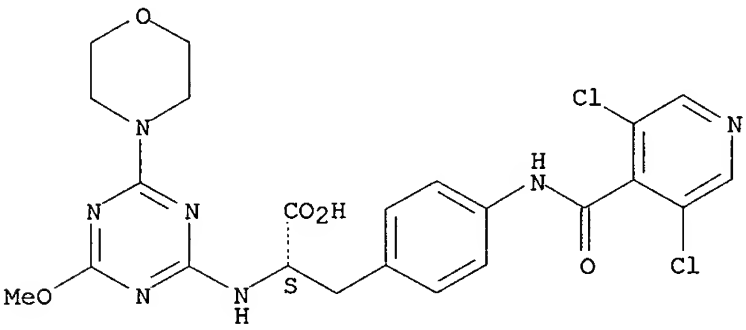
RN 263274-68-6 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[4-(diethylamino)-6-methoxy-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



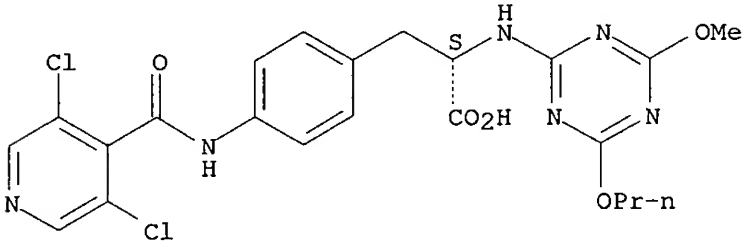
RN 263274-69-7 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[4-methoxy-6-(4-morpholinyl)-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



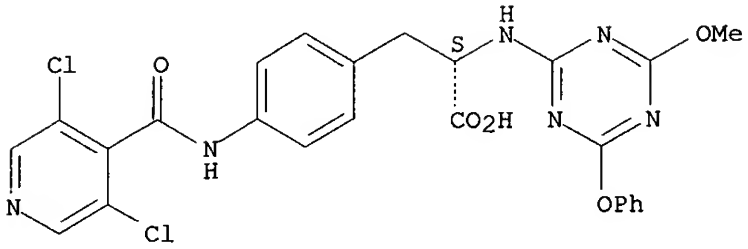
RN 263274-70-0 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-(4-methoxy-6-propoxy-1,3,5-triazin-2-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



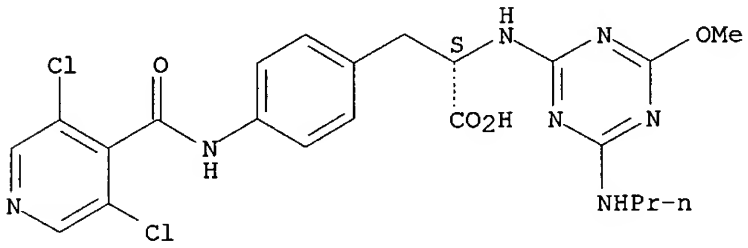
RN 263274-71-1 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-(4-methoxy-6-phenoxy-1,3,5-triazin-2-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



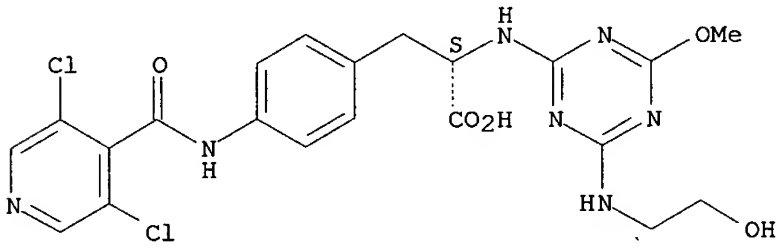
RN 263274-72-2 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[4-methoxy-6-(propylamino)-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



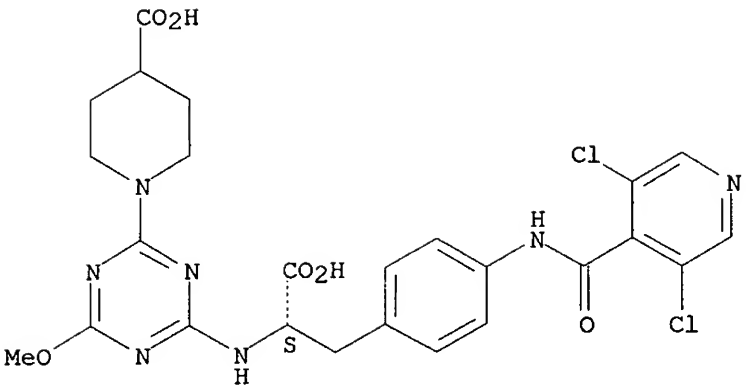
RN 263274-73-3 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[4-[(2-hydroxyethyl)amino]-6-methoxy-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



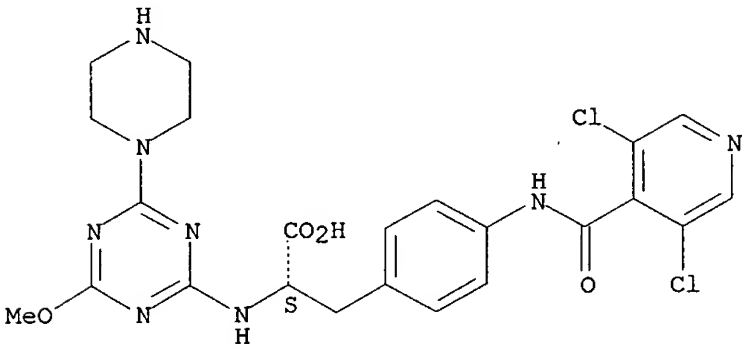
RN 263274-74-4 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[4-[[(1S)-1-carboxy-2-[4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]phenyl]ethyl]amino]-6-methoxy-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



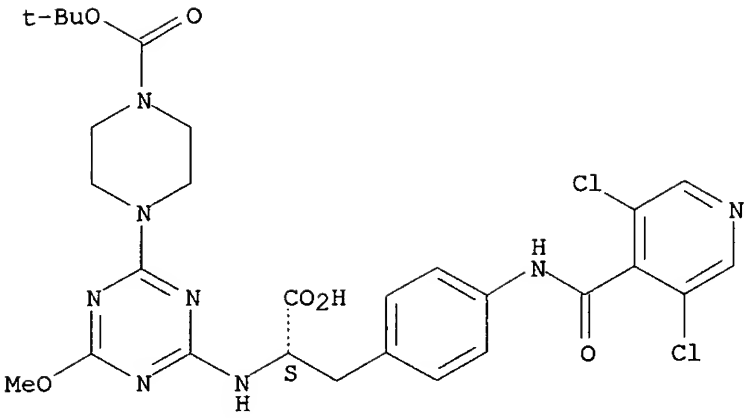
RN 263274-75-5 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[4-methoxy-6-(1-piperazinyl)-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



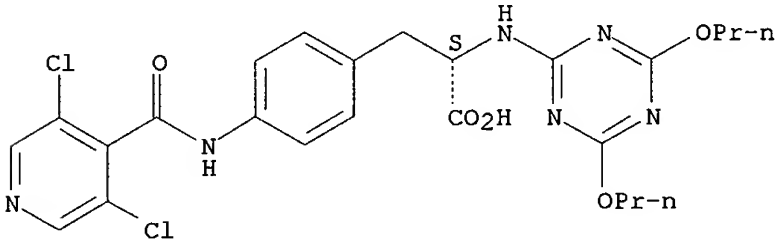
RN 263274-76-6 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[4-[[(1S)-1-carboxy-2-[4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]phenyl]ethyl]amino]-6-methoxy-1,3,5-triazin-2-yl]-, 1-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



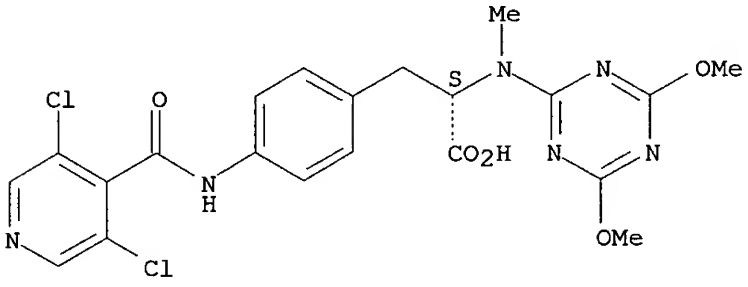
RN 263274-85-7 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-(4,6-dipropoxy-1,3,5-triazin-2-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



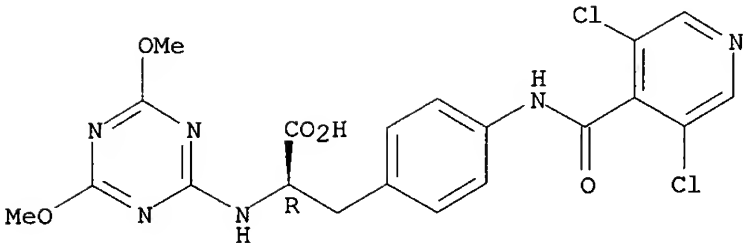
RN 263274-87-9 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-N-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



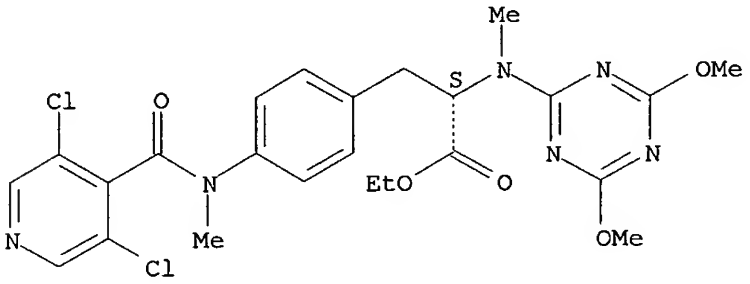
RN 263274-88-0 CAPLUS
CN D-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



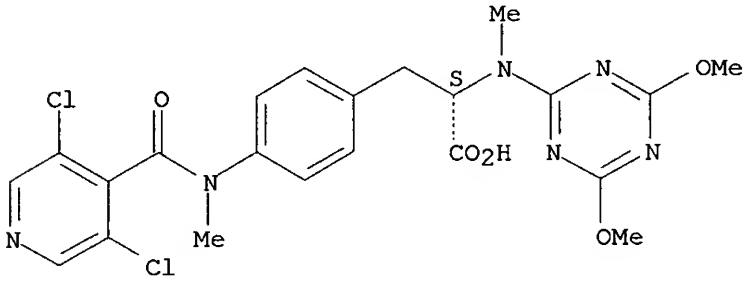
RN 263274-89-1 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]methylamino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-N-methyl-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



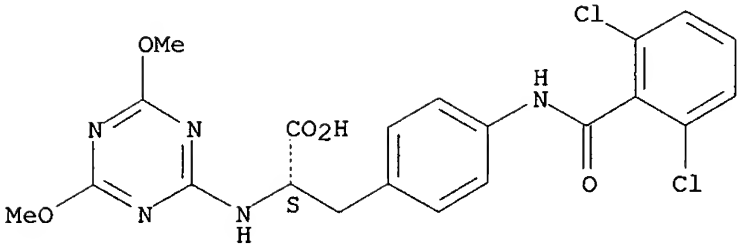
RN 263274-90-4 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]methylamino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-N-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



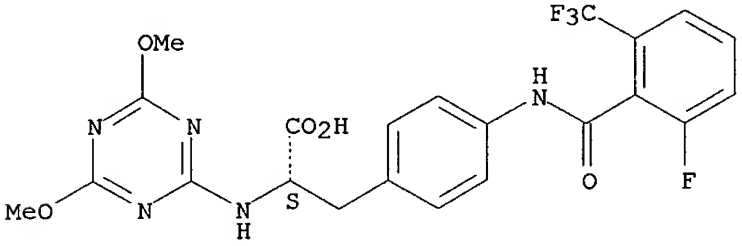
RN 263274-96-0 CAPLUS
CN L-Phenylalanine, 4-[(2,6-dichlorobenzoyl)amino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



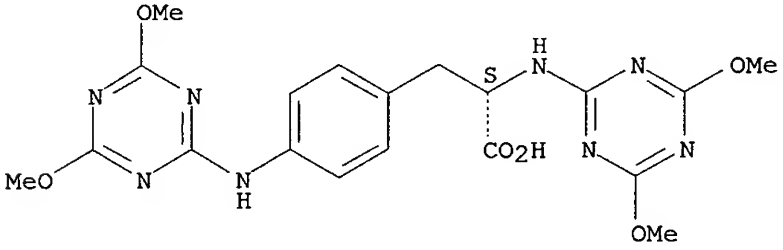
RN 263274-98-2 CAPLUS
CN L-Phenylalanine, N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-4-[[2-fluoro-6-(trifluoromethyl)benzoyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



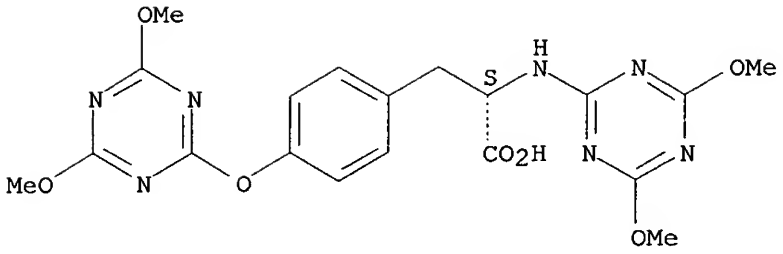
RN 263275-00-9 CAPLUS
CN L-Phenylalanine, N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-4-[(4,6-dimethoxy-1,3,5-triazin-2-yl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



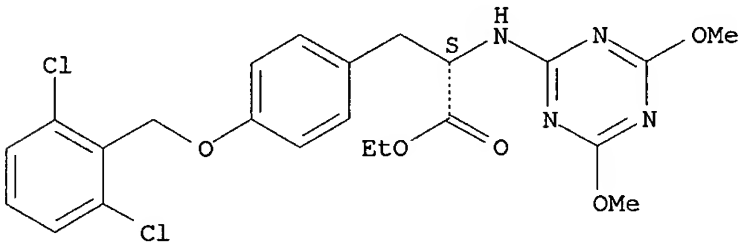
RN 263275-02-1 CAPLUS
CN L-Tyrosine, N,O-bis(4,6-dimethoxy-1,3,5-triazin-2-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



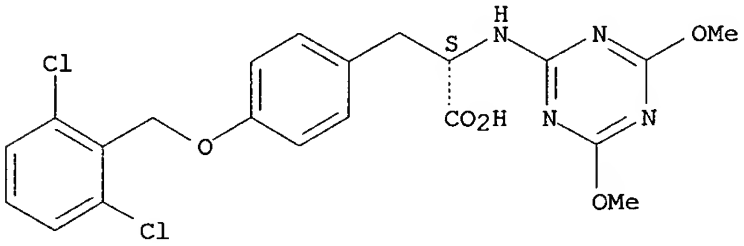
RN 263275-03-2 CAPLUS
CN L-Tyrosine, O-[(2,6-dichlorophenyl)methyl]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



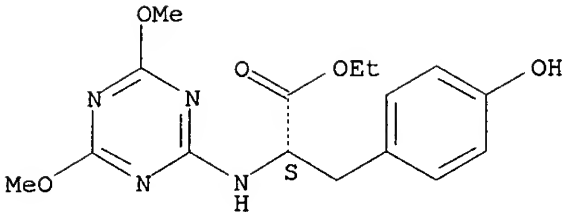
RN 263275-04-3 CAPLUS
CN L-Tyrosine, O-[(2,6-dichlorophenyl)methyl]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **263276-09-1P**
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of heteroaryl-.beta.-alanine derivs. as antiinflammatory agents and .alpha.4 integrin inhibitors)
RN 263276-09-1 CAPLUS
CN L-Tyrosine, N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.


OMe
O
OEt
OH
N
N
MeO
N
N
H
S

L18 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2002 ACS
AN 2002:90026 CAPLUS
DN 136:135019
TI Preparation of 3-amino-2-(4-aminocarbonyloxy)phenyl-propionic acid derivatives as antiinflammatory agents and .alpha.4 Integrin inhibitors
IN Konradi, Andrei W.; Pleiss, Michael A.; Thorsett, Eugene D.; Ashwell, Susan; Welmaker, Gregory S.; Kreft, Anthony; Sarantakis, Dimitrios; Dressen, Darren B.; Grant, Francine S.; Xu, Ying-Zi
PA Elan Pharmaceuticals, Inc., USA; American Home Products Corporation
SO PCT Int. Appl., 137 pp.
CODEN: PIXXD2
DT Patent
LA English

not prior art

FAN.CNT 1

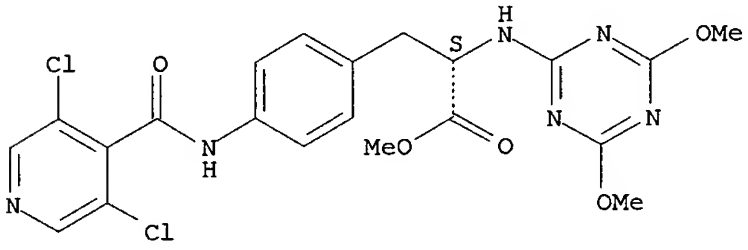
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2002008206	A1	20020131	WO 2001-US23073	20010720
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2002055509	A1	20020509	US 2001-910685	20010720
PRAI US 2000-220134P	P	20000721		

OS MARPAT 136:135019
AB 3-Amino-2-(4-aminocarbonyloxy)phenyl-propionic acid derivs. I wherein R is a carboxylic acid; R1 and R2 are independently selected from the group consisting of hydrogen, alkyl, substituted alkyl, alkenyl, substituted alkenyl, cycloalkyl, substituted cycloalkyl, or R1 and R2, together with the nitrogen atom to which they are attached, are joined to form an optionally substituted heterocyclic ring provided that said substituted alkyl, substituted alkenyl and substituted cycloalkyl do not carry an aryl, substituted aryl, heteroaryl or substituted heteroaryl group; Ra and R3 are independently a hydrogen or a Me group; R4 and R5 are independently selected from the group consisting of heteroatom group; n is zero or an integer 1; Alk is a straight or branched alkylene chain; Ar is an optionally substituted arom. or heteroarom. group, as well as their pharmaceutical use as .alpha.4.beta.7 Integrin inhibitors for the treatment of inflammatory diseases. Thus, 3-[4-(3,5-dichloropyrid-4-ylcarboxamido)phenyl]-2-(3-chlorophenylamino)propanoic acid was prepd. as .alpha.4 Integrin inhibitor. The preferred compds. of the invention generally have IC50 values in the .alpha.4.beta.1 and .alpha.a.beta.7 assays of 1 .mu.M and below. In the other assays featuring .alpha. integrins of other subgroups the same compds. had IC50 values of 50 .mu.M and above thus demonstrating the potency and selectivity of their action against .alpha.4 integrins. Title compds. were prepd. for treating an inflammatory condition in a mammalian patient which condition is mediated by Very Late Antigen 4 (VLA-4). Inflammatory condition is selected from the group consisting of asthma, Alzheimer's disease, **atherosclerosis**, AIDS dementia, diabetes, inflammatory bowel disease, multiple sclerosis, rheumatoid arthritis, tissue transplantation, tumor metastasis, meningitis, encephalitis, stroke, nephritis, retinitis, atopic dermatitis, psoriasis, myocardial ischemia and acute leukocyte-mediated lung injury.

IT **263274-37-9P 263274-66-4P 263274-86-8P**
263274-93-7P 263274-94-8P 263274-95-9P
263274-97-1P 263274-99-3P 263275-01-0P
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of aminoaminocarbonyloxyphenylpropionic acid derivs. as a integrin inhibitors)

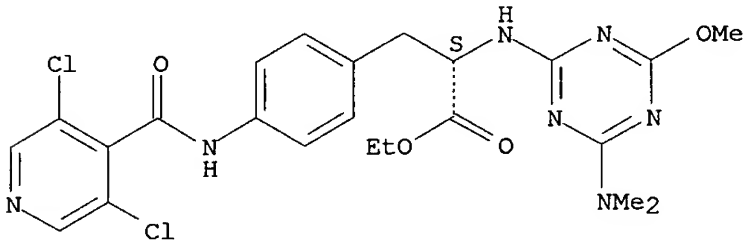
RN 263274-37-9 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



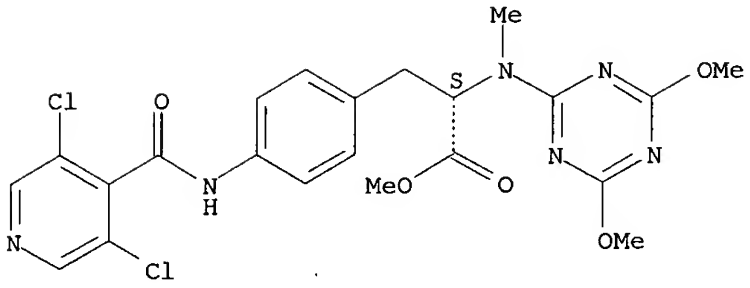
RN 263274-66-4 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[4-(dimethylamino)-6-methoxy-1,3,5-triazin-2-yl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



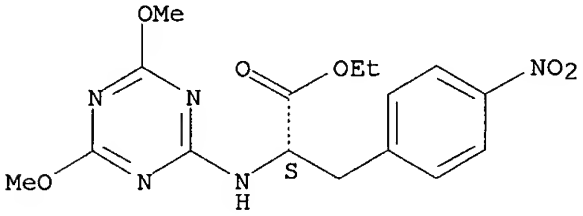
RN 263274-86-8 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-N-methyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



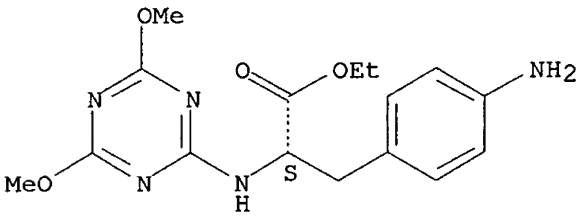
RN 263274-93-7 CAPLUS
CN L-Phenylalanine, N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-4-nitro-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



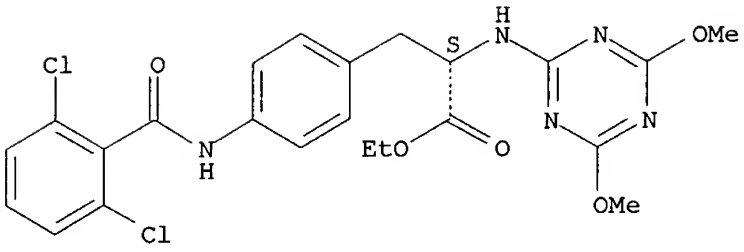
RN 263274-94-8 CAPLUS
CN L-Phenylalanine, 4-amino-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



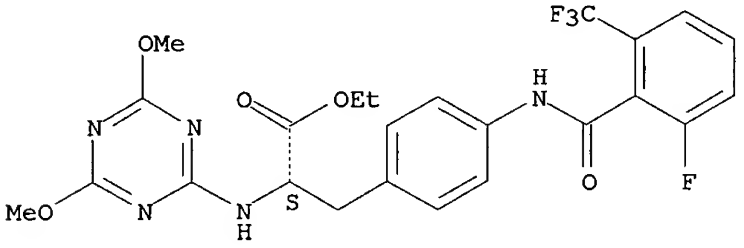
RN 263274-95-9 CAPLUS
CN L-Phenylalanine, 4-[(2,6-dichlorobenzoyl)amino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



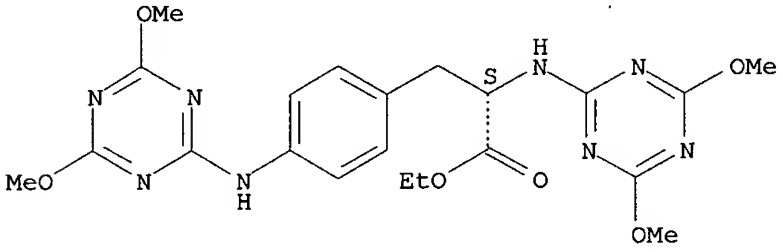
RN 263274-97-1 CAPLUS
CN L-Phenylalanine, N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-4-[[2-fluoro-6-(trifluoromethyl)benzoyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



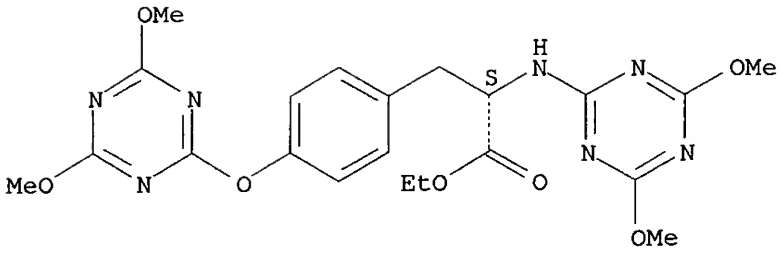
RN 263274-99-3 CAPLUS
CN L-Phenylalanine, N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-4-[(4,6-dimethoxy-1,3,5-triazin-2-yl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 263275-01-0 CAPLUS
CN L-Tyrosine, N,O-bis(4,6-dimethoxy-1,3,5-triazin-2-yl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

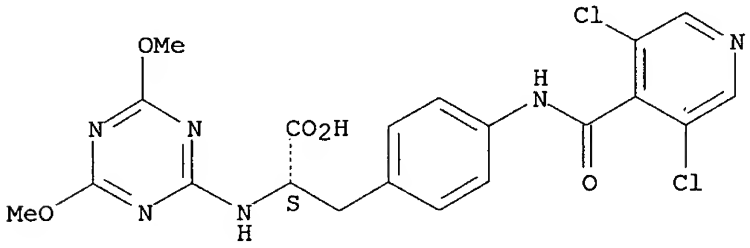


IT **263274-38-0P 263274-67-5P 263274-68-6P**
263274-69-7P 263274-70-0P 263274-71-1P
263274-72-2P 263274-73-3P 263274-74-4P
263274-75-5P 263274-76-6P 263274-85-7P
263274-87-9P 263274-88-0P 263274-89-1P
263274-90-4P 263274-96-0P 263274-98-2P
263275-00-9P 263275-02-1P 263275-03-2P
263275-04-3P
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of aminoaminocarbonyloxyphenylpropionic acid derivs. as a integrin inhibitors)

RN 263274-38-0 CAPLUS

CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)- (9CI) (CA INDEX NAME)

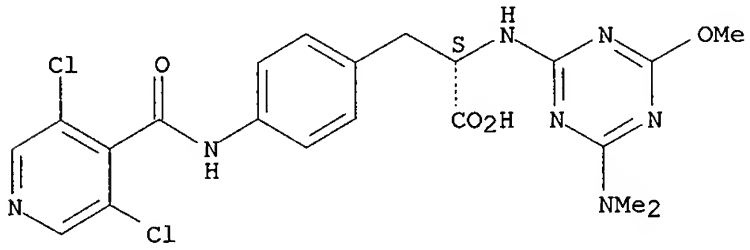
Absolute stereochemistry.



RN 263274-67-5 CAPLUS

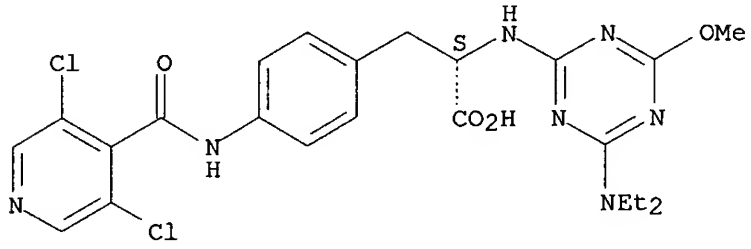
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[4-(dimethylamino)-6-methoxy-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



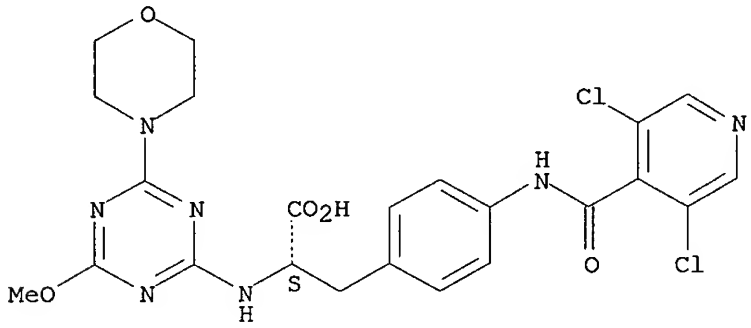
RN 263274-68-6 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[4-(diethylamino)-6-methoxy-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



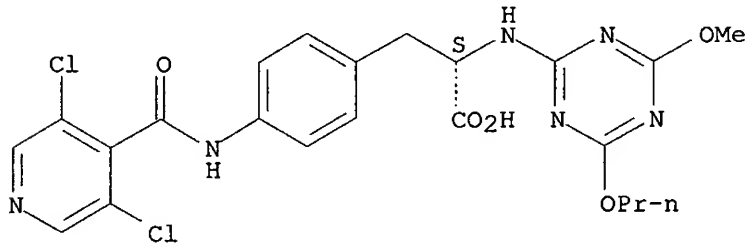
RN 263274-69-7 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[4-methoxy-6-(4-morpholinyl)-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



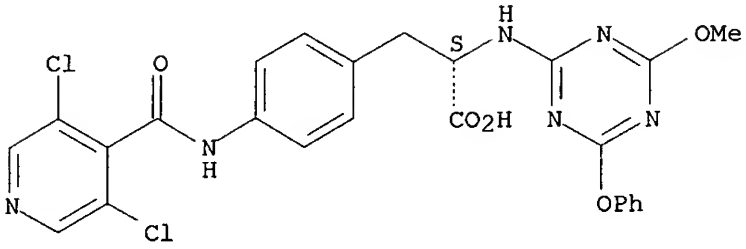
RN 263274-70-0 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-(4-methoxy-6-propoxy-1,3,5-triazin-2-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



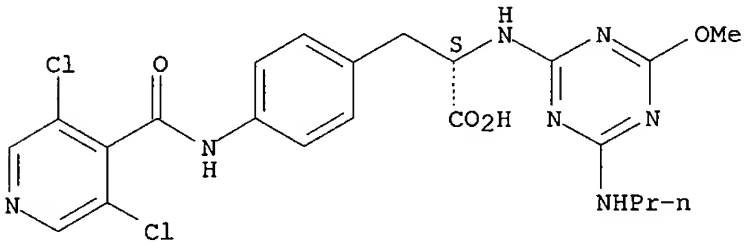
RN 263274-71-1 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-(4-methoxy-6-phenoxy-1,3,5-triazin-2-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



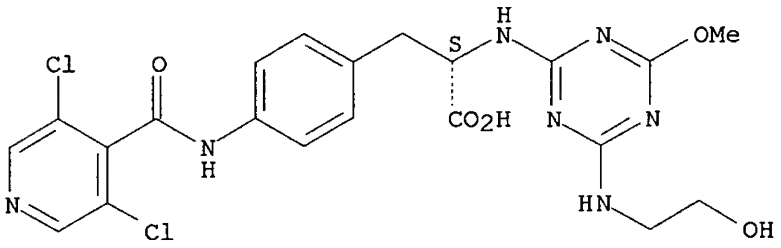
RN 263274-72-2 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[4-methoxy-6-(propylamino)-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



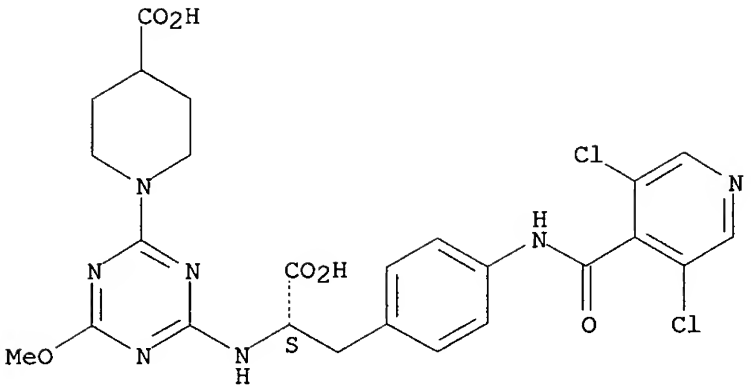
RN 263274-73-3 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[4-[(2-hydroxyethyl)amino]-6-methoxy-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



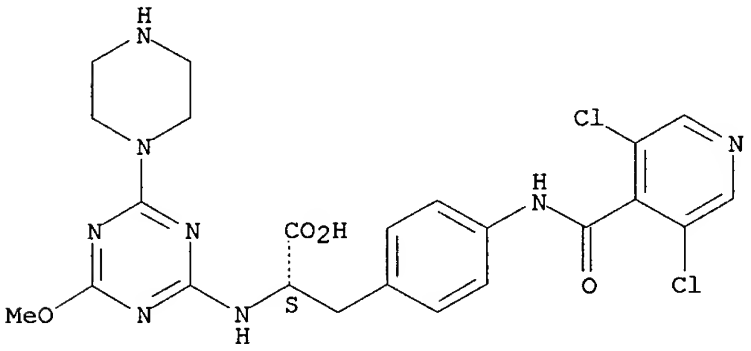
RN 263274-74-4 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[4-[[(1S)-1-carboxy-2-[4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]phenyl]ethyl]amino]-6-methoxy-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



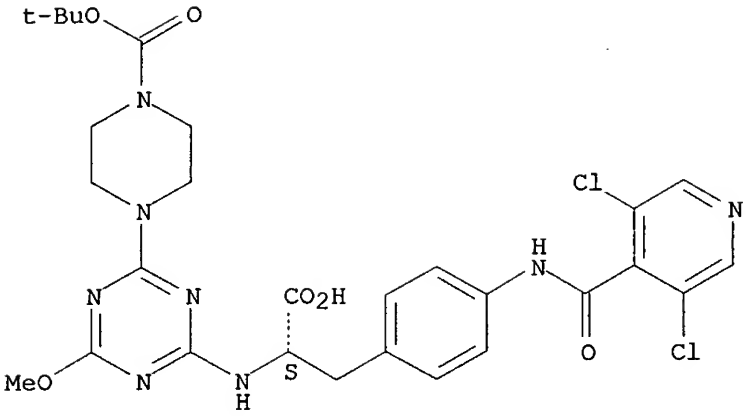
RN 263274-75-5 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[4-methoxy-6-(1-piperazinyl)-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



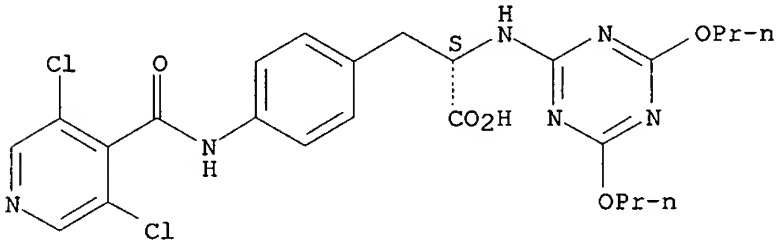
RN 263274-76-6 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[4-[[(1S)-1-carboxy-2-[4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]phenyl]ethyl]amino]-6-methoxy-1,3,5-triazin-2-yl]-, 1-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



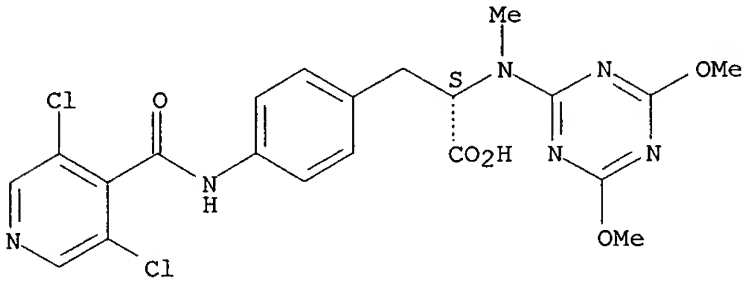
RN 263274-85-7 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-(4,6-dipropoxy-1,3,5-triazin-2-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



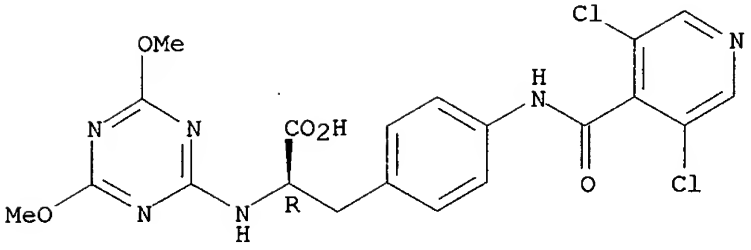
RN 263274-87-9 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-N-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



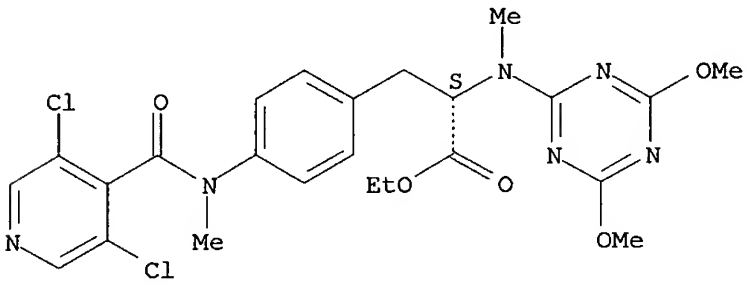
RN 263274-88-0 CAPLUS
CN D-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



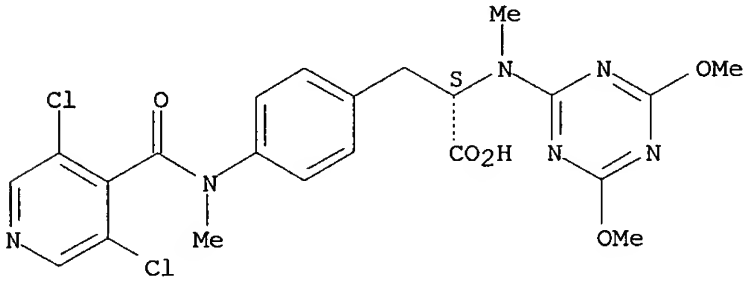
RN 263274-89-1 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]methylamino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-N-methyl-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



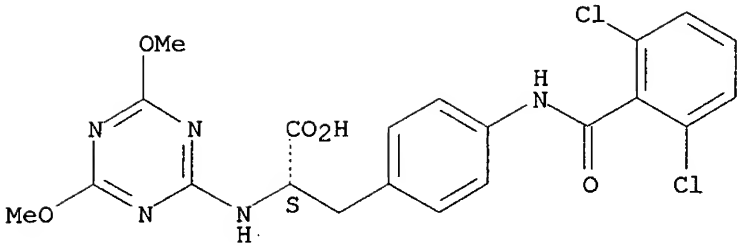
RN 263274-90-4 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]methylamino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-N-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



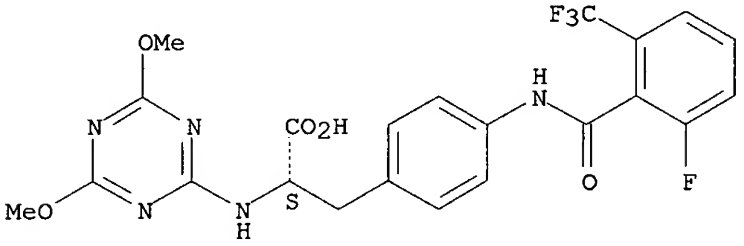
RN 263274-96-0 CAPLUS
CN L-Phenylalanine, 4-[(2,6-dichlorobenzoyl)amino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



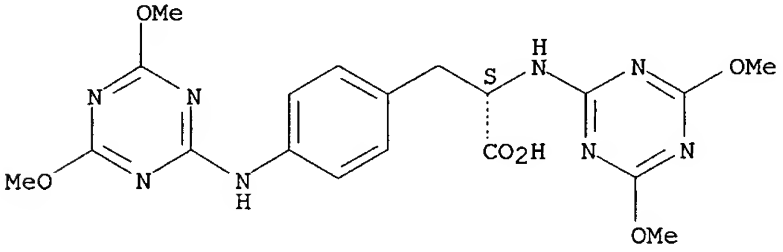
RN 263274-98-2 CAPLUS
CN L-Phenylalanine, N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-4-[[2-fluoro-6-(trifluoromethyl)benzoyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



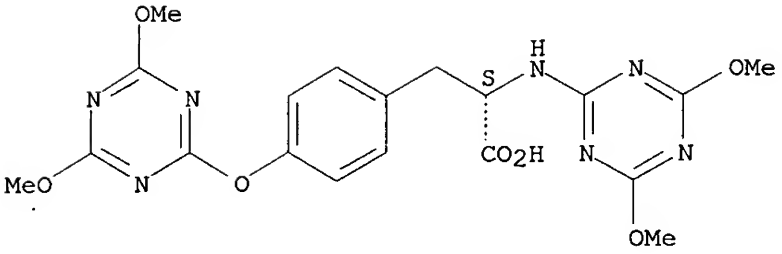
RN 263275-00-9 CAPLUS
CN L-Phenylalanine, N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-4-[(4,6-dimethoxy-1,3,5-triazin-2-yl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



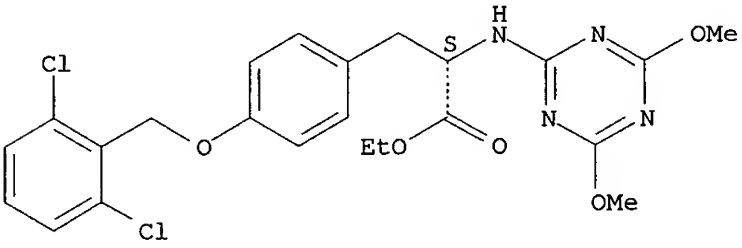
RN 263275-02-1 CAPLUS
CN L-Tyrosine, N,O-bis(4,6-dimethoxy-1,3,5-triazin-2-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



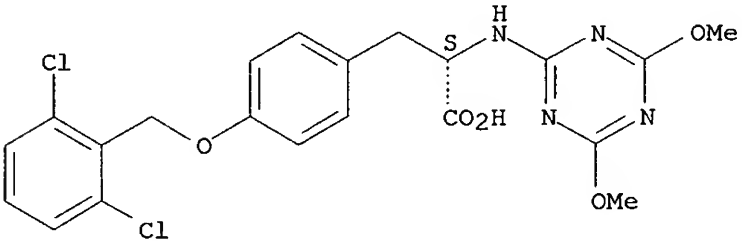
RN 263275-03-2 CAPLUS
CN L-Tyrosine, O-[(2,6-dichlorophenyl)methyl]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



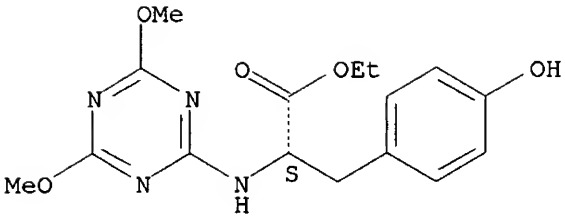
RN 263275-04-3 CAPLUS
CN L-Tyrosine, O-[(2,6-dichlorophenyl)methyl]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



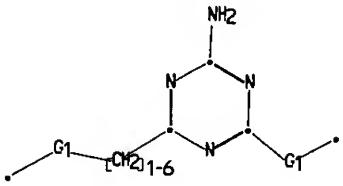
IT **263276-09-1P**
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of aminoaminocarbonyloxyphenylpropionic acid derivs. as a integrin inhibitors)
RN 263276-09-1 CAPLUS
CN L-Tyrosine, N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-, ethyl ester (9CI) (CA INDEX NAME)

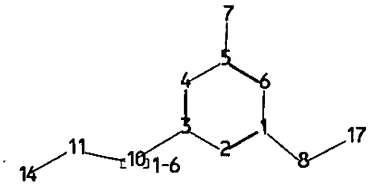
Absolute stereochemistry.



RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

C:\STNEXP4\QUERIES\10005064 (ex2).str



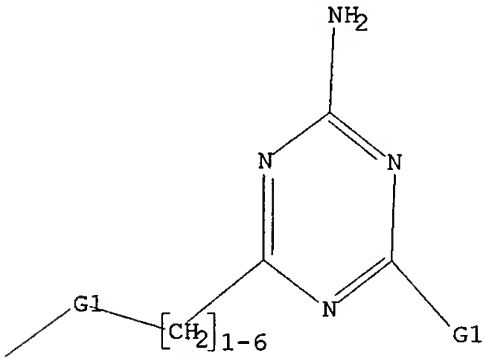


chain nodes :
8 10 11
ring nodes :
1 2 3 4 5 6
ring/chain nodes :
7 14 17
chain bonds :
1-8 3-10 5-7 8-17 10-11 11-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-8 5-7 8-17 10-11 11-14
exact bonds :
3-10
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:O,S,N

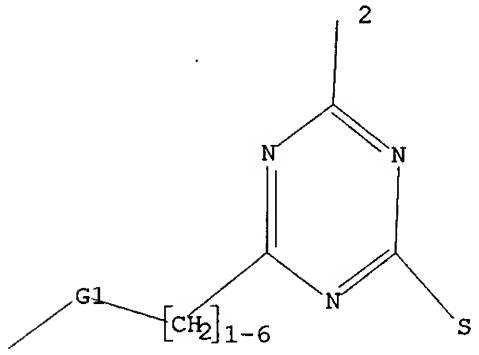
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 10:CLASS 11:CLASS
14:CLASS 17:CLASS

```
=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 2016 OR  2026 OR  2039 OR  2040

L1    SCREEN CREATED

=>
Uploading C:\STNEXP4\QUERIES\10005064 (ex2).str

L2      STRUCTURE UPLOADED

=> que L2 NOT L1

L3   QUE L2 NOT L1

=> d l3
L3 HAS NO ANSWERS
L1               SCR 2016 OR 2026 OR 2039 OR 2040
L2               STR
```




```
G1 O,S,N


Structure attributes must be viewed using STN Express query preparation.
L3               QUE  L2 NOT L1


=> s l3 sss sam
SAMPLE SEARCH INITIATED 17:40:32 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    862 TO ITERATE

100.0% PROCESSED     862 ITERATIONS                          20 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        15479 TO    19001
PROJECTED ANSWERS:             132 TO      668

L4           20 SEA SSS SAM L2 NOT L1
```

```
=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 2016 OR  2026 OR  2039 OR  2040

L5    SCREEN CREATED

=>
Uploading C:\STNEXP4\QUERIES\10005064 (ex2).str

L6      STRUCTURE UPLOADED

=> que L6 NOT L5

L7   QUE L6 NOT L5

=> d l7
L7 HAS NO ANSWERS
L5              SCR 2016 OR 2026 OR 2039 OR 2040
L6              STR
```




```
G1 O,S,N


Structure attributes must be viewed using STN Express query preparation.
L7              QUE  L6 NOT L5


=> s l7 sss sam
SAMPLE SEARCH INITIATED 17:42:46 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     28 TO ITERATE

100.0% PROCESSED      28 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          243 TO      877
PROJECTED ANSWERS:               0 TO        0

L8            0 SEA SSS SAM L6 NOT L5

=> ....Testing the current file.... screen
```

ENTER SCREEN EXPRESSION OR (END):end

=> screen 2016 OR 2026 OR 2039 OR 2040

L9 SCREEN CREATED

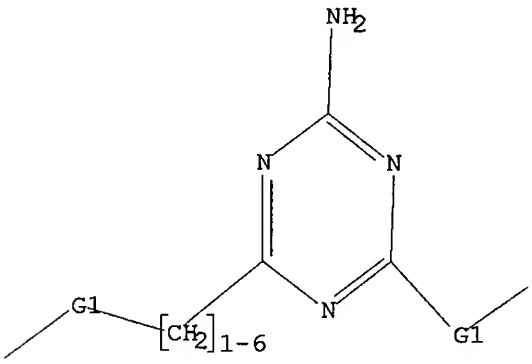
=>
Uploading C:\STNEXP4\QUERIES\10005064 (ex2).str

L10 STRUCTURE UPLOADED

=> que L10 NOT L9

L11 QUE L10 NOT L9

=> d l11
L11 HAS NO ANSWERS
L9 SCR 2016 OR 2026 OR 2039 OR 2040
L10 STR



G1 O,S,N

Structure attributes must be viewed using STN Express query preparation.
L11 QUE L10 NOT L9

=> s l11 sss sam
SAMPLE SEARCH INITIATED 17:44:38 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 696 TO ITERATE

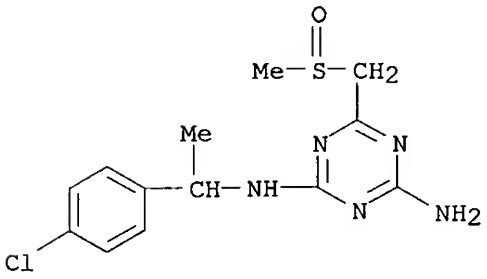
100.0% PROCESSED 696 ITERATIONS 7 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 12338 TO 15502
PROJECTED ANSWERS: 7 TO 298

L12 7 SEA SSS SAM L10 NOT L9

=> d scan l12

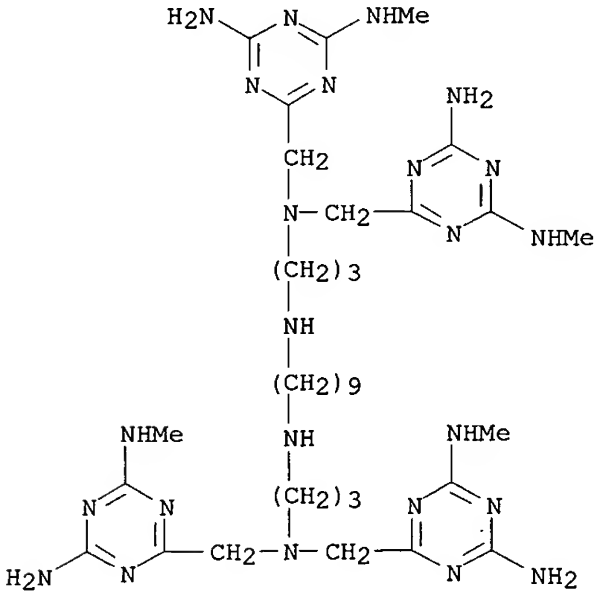
L12 7 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1,3,5-Triazine-2,4-diamine, N-[1-(4-chlorophenyl)ethyl]-6-[(methylsulfinyl)methyl]- (9CI)
MF C13 H16 Cl N5 O S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

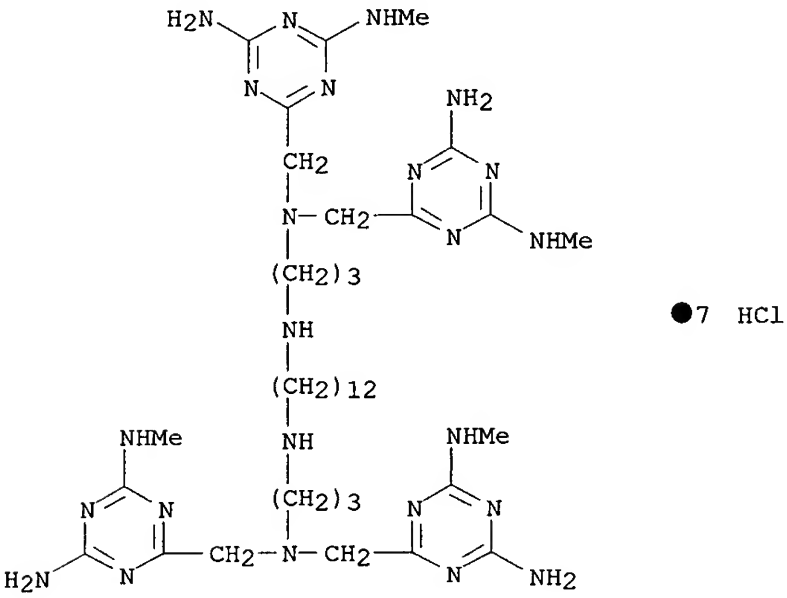
```
=> s l11 sss ful
FULL SEARCH INITIATED 17:45:27 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  13319 TO ITERATE

100.0% PROCESSED   13319 ITERATIONS                          187 ANSWERS
SEARCH TIME: 00.00.03

L13          187 SEA SSS FUL L10 NOT L9

=> s l13
L14           38 L13

=> d l14 1-38 bib,ab,hitstr
```

L14 ANSWER 1 OF 38 CAPLUS COPYRIGHT 2002 ACS
AN 2001:680366 CAPLUS
DN 135:366327
TI Synthesis and Biological Evaluation of s-Triazine Substituted Polyamines as Potential New Anti-Trypanosomal Drugs
AU Klenke, Burkhard; Stewart, Mhairi; Barrett, Michael P.; Brun, Reto; Gilbert, Ian H.
CS Welsh School of Pharmacy, Cardiff University, Cardiff, CF10 3XF, UK
SO Journal of Medicinal Chemistry (2001), 44(21), 3440-3452
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB The P2 transporter is a nucleoside transporter which is unique to the protozoan parasite Trypanosoma brucei, the causative organism of Human African Trypanosomiasis. The transporter has been shown to bind some structural motifs not recognized by other transporters. In this paper we describe the use of the melamine motif, a substrate of the P2 transporter, as a potential tool to selectively deliver polyamine analogs to the parasites. The synthesis of a no. of polyamine analogs attached to a variety of melamine analogs is described. Many of the compds. were shown to competitively inhibit uptake of adenosine, indicating that they are recognized by the transporter. Some of the compds. showed good in vitro activity against the parasites.
IT **374674-07-4P 374674-10-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. and structure activity relationships of s-triazine substituted polyamines as antitrypanosomal drugs)
RN 374674-07-4 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6,6',6'',6'''-[1,9-nonanediylbis[imino-3,1-propanediylnitrilobis(methylene)]]tetrakis[N-methyl-, heptahydrochloride (9CI) (CA INDEX NAME)



●7 HCl

RN 374674-10-9 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6,6',6'',6'''-[1,12-dodecanediylbis[imino-3,1-propanediylnitrilobis(methylene)]]tetrakis[N-methyl-, heptahydrochloride (9CI) (CA INDEX NAME)



●7 HCl

RE.CNT 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 2 OF 38 CAPLUS COPYRIGHT 2002 ACS
AN 2001:453092 CAPLUS
DN 135:61555
TI Preparation of lipopeptides as antibacterial agents
IN Hill, Jason; Parr, Ian; Morytko, Michael; Siedlecki, Jim; Yu, Xiang Yang; Silverman, Jared; Keith, Dennis; Finn, John; Christensen, Dale; Lazarova, Tsvetelina; Watson, Alan D.; Zhang, Yan
PA Cubist Pharmaceuticals, Inc., USA; et al.
SO PCT Int. Appl., 202 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

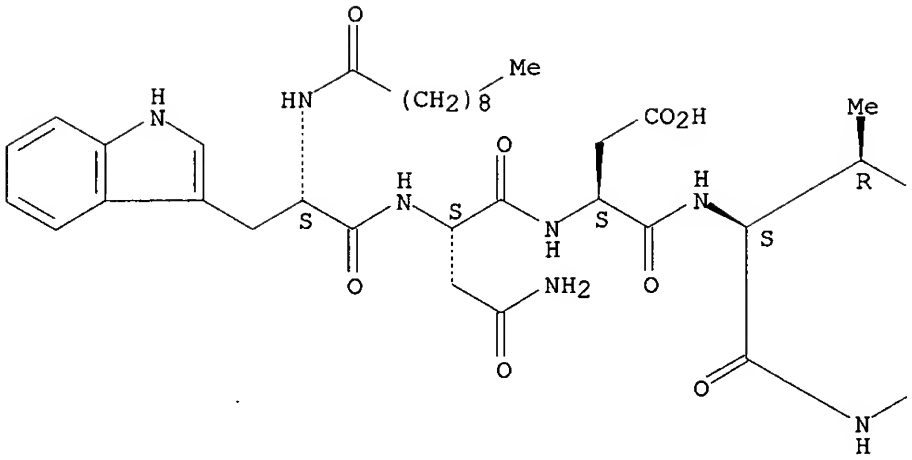
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2001044274	A1	20010621	WO 2000-US34205	20001215

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

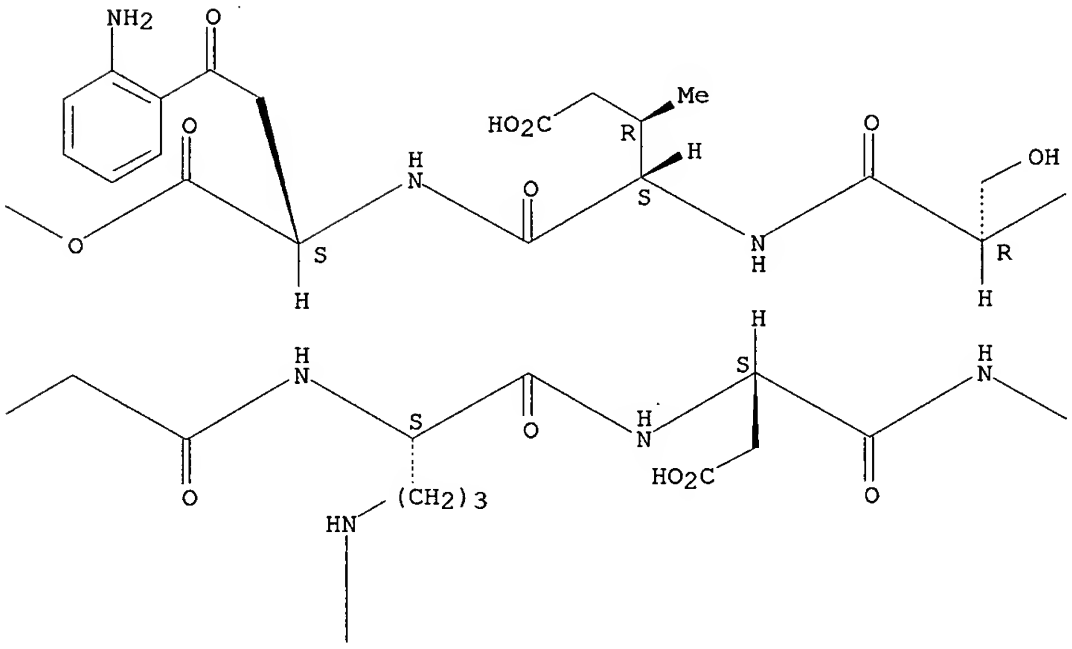
PRAI US 1999-170946P P 19991215
US 2000-208222P P 20000530
OS MARPAT 135:61555
AB Lipopeptides I [R is -N(B)(X)n-A; B is X''RY, H, alkyl, alkenyl, alkynyl, aryl, heteroaryl, cycloalkyl or heterocyclyl; RY is hydrido, alkyl, alkenyl, alkynyl, aryl, heteroaryl, cycloalkyl, heterocyclyl or hydroxyl; X, X'' are C:O, C:S, C:NH, C:NRX, S:O or SO2; n is 0 or 1; RX is alkyl, alkenyl, alkynyl, aryl, heteroaryl, cycloalkyl, heterocyclyl, hydroxyl, alkoxy, carboxy or carboalkoxy; A is H, NH2, NHRA, NRARB, heteroaryl, cycloalkyl, heterocyclyl (RA, RB are alkyl, alkenyl, alkynyl, aryl, heteroaryl, cycloalkyl, heterocyclyl or carboalkoxy) or when n is 0, then A is P(O)(OR50)OR51, P(O)R52R53, or P(O)(OR50)R53, where R50-R53 are alkyl; alternatively B and A may form a 5-7 membered heterocyclic or heteroaryl ring; R1 is defined similarly to R (with provisos); R2 is CH2CR17R18-ring, where R17 and R18 are hydrido, halo, hydroxyl, alkoxy, amino, thio, sulfinyl, sulfonyl, etc. or CR17R18 are CO, C(:S), oxime or hydrazone group] were prepd. for use as antibacterials. Thus, treating daptomycin with 4-fluorobenzaldehyde and sodium triacetoxyborohydride in dry DMF for 24 h afforded I [R = NHCO(CH2)8Me, R1 = NHCH2C6H4F-4, R2 = CH2COC6H4NH2-o], which showed MIC (S. Aureus) .ltoreq. 1 .mu.g/mL.
IT **345643-87-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of lipopeptides as antibacterial agents)
RN 345643-87-0 CAPLUS
CN Daptomycin, 6-[N5-[[4-amino-6-(phenylamino)-1,3,5-triazin-2-yl]methyl]-L-ornithine]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

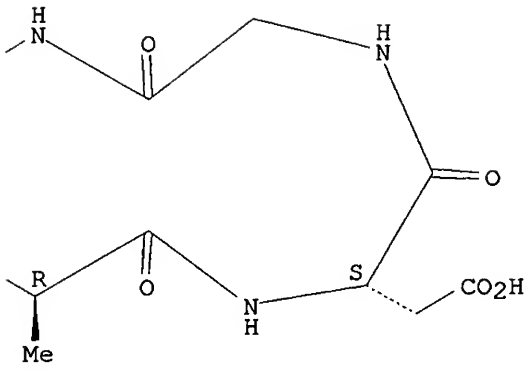
PAGE 1-A



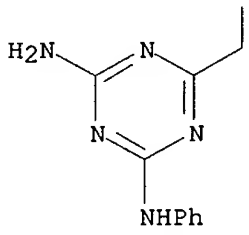
PAGE 1-B



PAGE 1-C

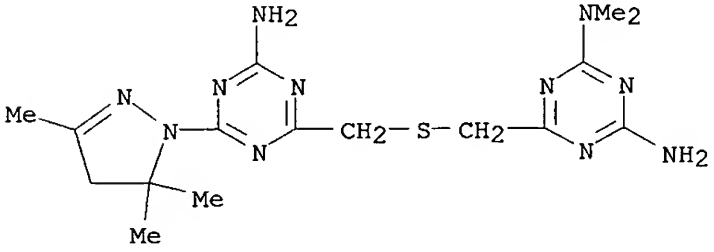


PAGE 2-B



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 3 OF 38 CAPLUS COPYRIGHT 2002 ACS
AN 2001:87180 CAPLUS
DN 134:311186
TI Synthesis, structural characterization and antitumor activity of novel 2,4-diamino-1,3,5-triazine derivatives
AU Brzozowski, Z.; Saczewski, F.; Gdaniec, M.
CS Department of Chemical Technology of Drugs, Medical University of Gdansk, Gdansk, P-80-416, Pol.
SO European Journal of Medicinal Chemistry (2000), 35(12), 1053-1064
CODEN: EJMCA5; ISSN: 0223-5234
PB Editions Scientifiques et Medicales Elsevier
DT Journal
LA English
AB The syntheses, structural elucidation and antitumor activities of novel 2,4-diamino-1,3,5-triazine derivs. are described. The crystal structure of one compd., 4-(chloromethyl)-6-(4,5-dihydro-3,5,5-trimethyl-1H-pyrazol-1-yl)-1,3,5-triazin-2-amine, was reported. Screenings performed at NCI showed that most derivs. possessed a moderate to strong growth inhibition activity on various tumor panel cell lines between 0.148 and 56.2 .mu.M concns. 4-(Chloromethyl)-6-(4,5-dihydro-3,5,5-trimethyl-1H-pyrazol-1-yl)-1,3,5-triazin-2-amine showed the most potent antitumor activity with the mean midpoint values of log10 GI50, log10 TGI50 and Log10 LC50 of all tests equal to -5.26, -4.81 and -4.37, resp. and therefore, it can be considered as a lead structure for further development of anticancer agents.
IT **334993-93-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of antitumor diaminotriazines via cyclization of biguanides with alkanoic acid esters)
RN 334993-93-0 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6-[[[[4-amino-6-(4,5-dihydro-3,5,5-trimethyl-1H-pyrazol-1-yl)-1,3,5-triazin-2-yl]methyl]thio]methyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)



RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

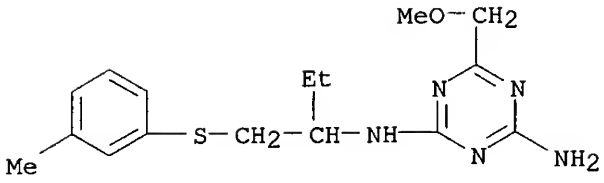
L14 ANSWER 5 OF 38 CAPLUS COPYRIGHT 2002 ACS
AN 1999:626180 CAPLUS
DN 131:243289
TI Preparation of 2-[(2-arylthioethyl)amino]-4-amino-1,3,5-triazines as herbicides
IN Kirsten, Rolf; Riebel, Hans-Jochem; Lehr, Stefan; Voigt, Katharina; Kather, Kristian; Dollinger, Markus; Drewes, Mark Wilhelm; Wetcholowsky, Ingo; Watanabe, Yukiyoshi; Goto, Toshio; Myers, Randy Allen
PA Bayer Aktiengesellschaft, Germany; Nihon Bayer Agrochem K.K.
SO PCT Int. Appl., 121 pp.
CODEN: PIXXD2
DT Patent
LA German

Provisional #2

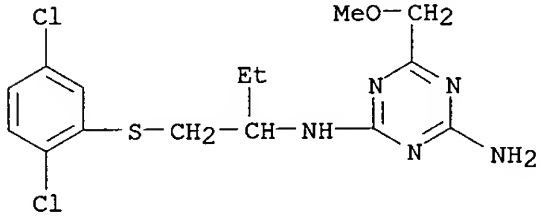
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9948877	A1	19990930	WO 1999-EP1559	19990311
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
DE 19812879	A1	19990930	DE 1998-19812879	19980324
CA 2325489	AA	19990930	CA 1999-2325489	19990311
AU 9929328	A1	19991018	AU 1999-29328	19990311
EP 1064271	A1	20010103	EP 1999-910340	19990311
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL				
PRAI DE 1998-19812879	A	19980324		
WO 1999-EP1559	W	19990311		

OS MARPAT 131:243289
AB Title compds. [I; n = 0, 1, 2; R1 = H, (substituted) alkyl; R2 = H, formyl, (substituted) alkyl, alkylcarbonyl, alkoxycarbonyl; R3 = (substituted) alkyl, cycloalkyl; R4 = H, alkyl; Ar = (substituted) Ph, naphthyl, heterocyclyl; Z = H, (substituted) alkyl, alkylcarbonyl, alkoxycarbonyl, alkenyl, alkynyl, cycloalkyl], were prepd. Thus, 1-[1-(3-methylphenylthiomethyl)propyl]biguanide hydrochloride and zeolite mol. sieves in MeOH at -10.degree. were treated with NaOMe and Me methoxyacetate followed by 15 h stirring to give 70% 2-amino-4-methoxymethyl-6-[1-(3-methylphenylthiomethyl)propylamino]-1,3,5-triazine. Several I at 250-1000 g/ha preemergent gave complete control of Solanum, Digitaria, Chenopodium, Veronica, etc.
IT **244264-98-0P 244264-99-1P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 2-[(2-arylthioethyl)amino]-4-amino-1,3,5-triazines as herbicides)
RN 244264-98-0 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6-(methoxymethyl)-N-[1-[[(3-methylphenyl)thio]methyl]propyl]- (9CI) (CA INDEX NAME)



RN 244264-99-1 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, N-[1-[[(2,5-dichlorophenyl)thio]methyl]propyl]-6-(methoxymethyl)- (9CI) (CA INDEX NAME)



RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 6 OF 38 CAPLUS COPYRIGHT 2002 ACS
AN 1999:238562 CAPLUS
DN 130:296699
TI Preparation of 2,4-diamino-1,3,5-triazines as herbicides
IN Riebel, Hans-Jochem; Lehr, Stefan; Stelzer, Uwe; Dollinger, Markus; Drewes, Mark Wilhelm; Myers, Randy Allen
PA Bayer A.-G., Germany
SO Ger. Offen., 36 pp.
CODEN: GWXXBX
DT Patent
LA German

Proviso #2

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI DE 19744232	A1	19990408	DE 1997-19744232	19971007
CA 2305806	AA	19990415	CA 1998-2305806	19980924
WO 9918100	A1	19990415	WO 1998-EP6098	19980924
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9896280	A1	19990427	AU 1998-96280	19980924
AU 742963	B2	20020117		
EP 1021441	A1	20000726	EP 1998-950080	19980924
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL				
BR 9812892	A	20000808	BR 1998-12892	19980924
JP 2001519348	T2	20011023	JP 2000-514911	19980924
US 6348435	B1	20020219	US 2000-508383	20000501
PRAI DE 1997-19744232	A	19971007		
WO 1998-EP6098	W	19980924		

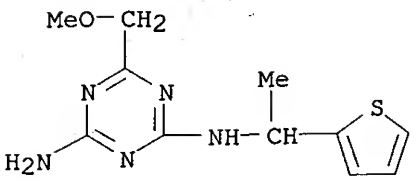
OS MARPAT 130:296699

AB The title compds. [I; R1 = H, (un)substituted C1-6 alkyl; R2 = H, (un)substituted C1-6 alkyl, COR6; R3 = H, (un)substituted C1-6 alkyl, (un)substituted C2-6 alkenyl or alkynyl, etc; R4 = H, (un)substituted C1-6 alkyl, H, (un)substituted C3-6 cycloalkyl; R5 = H, (un)substituted furyl or thienyl; R6 = (un)substituted C1-6 alkyl(amino), alkoxy, etc.] were prepd., e.g., by reaction of biguanides R1R2NC(:NH)NHC(:NH)NHCR4R5 (R1, R2, R4, R5 as above) or their acid adducts, with alkoxycarbonyl compds. RO2CR3 (R = alkyl, R3 as above). For example, N-deformylation of N-[1-(thien-2-yl)ethyl]formamide (prepn. in 64% yield from 2-acetylthiophene, HCO2H and H2NCHO given) by refluxing with aq. HCl gave 41% 1-(thien-2-yl)ethylamine which was condensed with cyanoguanidine to give 99% 1-[1-(thien-2-yl)ethyl]biguanide.cntdot.HCl. Cyclocondensation of the latter with EtCO2Me in MeOH in the presence of NaOMe gave 32% 2-amino-4-ethyl-6-[1-(thien-2-yl)ethyl]amino-1,3,5-triazine which was N-acetylated with Ac2O to give 45% of a title triazine I (R1 = H, R2 = R4 = Me, R3 = Et, R5 = 2-thienyl) (m. 153.degree.).

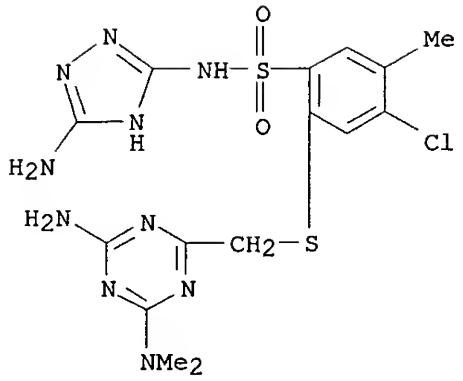
IT **223142-23-2P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 2,4-diamino-1,3,5-triazines as herbicides)

RN 223142-23-2 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6-(methoxymethyl)-N-[1-(2-thienyl)ethyl]-

(9CI) (CA INDEX NAME)

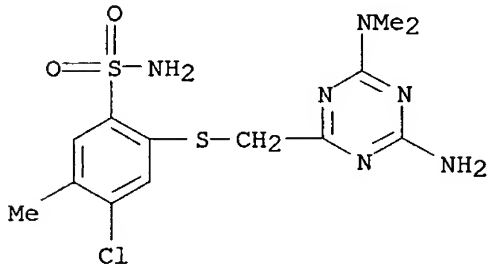


L14 ANSWER 13 OF 38 CAPLUS COPYRIGHT 2002 ACS
AN 1997:762561 CAPLUS
DN 128:97298
TI 2-Mercaptobenzenesulfonamides as novel inhibitors of human immunodeficiency virus type 1 integrase and replication
AU Neamati, N.; Mazumder, A.; Sunder, S.; Owen, J. M.; Schultz, R. J.; Pommier, Y.
CS Lab. Mol. Pharmacol., Div. Basic Sci., Natl. Cancer Inst., Bethesda, MD, 20892, USA
SO Antiviral Chem. Chemother. (1997), 8(6), 485-495
CODEN: ACCHEH; ISSN: 0956-3202
PB International Medical Press
DT Journal
LA English
AB An obligatory requirement in the retroviral life cycle is the integration of the viral dsDNA into the host chromosome, a process performed by viral integrase. The retroviral integrase is able to catalyze at least three discrete enzymic steps. Two of these steps, 3' processing and DNA strand transfer, can be measured in an in vitro assay in the presence of a duplex oligonucleotide corresponding to the viral long terminal repeat, recombinant integrase and the divalent cations, Mg2+ or Mn2+. This assay provides an efficient means of testing integrase inhibitors. As part of our continuous effort in developing novel inhibitors we examd. a series of 2-mercaptobenzenesulfonamides (MBSAs) for their inhibitory activity against human immunodeficiency virus type 1 (HIV-1) integrase. From the list of compds. tested in an assay specific for HIV-1 integrase, 26 compds. inhibited the 3' processing and strand transfer step with 50% inhibitory concn. (IC50) values below 25 .mu.M. All the thioether derivs. were inactive. These results were further compared with the ability of MBSAs to protect HIV-1-infected T4 lymphocyte CEM cells. Among 68 compds. tested, 27 exhibited antiviral activity in cell-based assays with therapeutic indexes of 1-16. All the MBSAs with antiviral activity were also effective inhibitors of recombinant HIV-1 integrase. Several arom. disulfides were also tested and found to exhibit moderate antiviral and anti-integrase activities. These data demonstrate that MBSAs can be developed as inhibitors of HIV-1 integrase with the potential for antiviral activity.
IT **201229-86-9**, NSC 661081 **201229-87-0**, NSC 661082
RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)
(structure-activity relations of mercaptobenzenesulfonamides as novel inhibitors of HIV-1 integrase and replication)
RN 201229-86-9 CAPLUS
CN Benzenesulfonamide, 2-[[[4-amino-6-(dimethylamino)-1,3,5-triazin-2-yl]methyl]thio]-N-(5-amino-1H-1,2,4-triazol-3-yl)-4-chloro-5-methyl- (9CI) (CA INDEX NAME)



Previous (new)

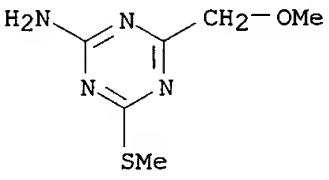
RN 201229-87-0 CAPLUS
CN Benzenesulfonamide, 2-[[[4-amino-6-(dimethylamino)-1,3,5-triazin-2-yl]methyl]thio]-4-chloro-5-methyl- (9CI) (CA INDEX NAME)



L14 ANSWER 17 OF 38 CAPLUS COPYRIGHT 2002 ACS
AN 1990:532221 CAPLUS
DN 113:132221
TI Preparation of N-arylsulfonyl-N'-triazinylurea derivatives as herbicides
IN Levitt, George
PA du Pont de Nemours, E. I., and Co., USA
SO U.S., 74 pp. Cont.-in-part of U.S. 4,305,884.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 8

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4892946	A	19900109	US 1980-209307	19801124
	US 4394506	A	19830719	US 1979-98781	19791130
	US 4305884	A	19811215	US 1980-171355	19800723
	AU 547325	B2	19851017	AU 1983-13286	19830408
	AU 8313286	A1	19830804		
PRAI	US 1979-98781		19791130		
	US 1980-171355		19800723		
	US 1978-910965		19780530		
	US 1978-965070		19781130		
	US 1979-15341		19790301		
	US 1979-29281		19790413		
	AU 1979-47545		19790529		
	US 1979-49149		19790618		
	US 1980-119165		19800206		

OS MARPAT 113:132221
AB The title urea derivs. [I; R = C1-12 alkoxy, C3-10 alkenyloxy, alkynyloxy, 1-indolinyl, etc.; R2 = NCO, CF3SO2NH, etc.; R3 = H, Me, Cl, Br, F; W = O, S; X = H, Cl, Me, alkoxy, etc.; Y = H, F, Cl, Br, C1-4 alkyl, etc.; Z = N, CH] are prepd. and are useful as herbicides. To a soln. of isocyanate deriv. II in MeCN was added in small portions at room temp. triazine deriv. III to give the urea deriv. I (R = X = MeO, R2 = 5-NCO, R3 = H, W = O, Y = Me, Z = N). Among approx. 50 I prepd. 20 were tested to show pre- and post-emergent herbicidal activity at 0.05 g/ha against a wide variety of weeds.
IT **129346-28-7**
RL: PROC (Process)
(addn. of, with benzenesulfonyl isocyanate deriv.)
RN 129346-28-7 CAPLUS
CN 1,3,5-Triazin-2-amine, 4-(methoxymethyl)-6-(methylthio)- (9CI) (CA INDEX NAME)

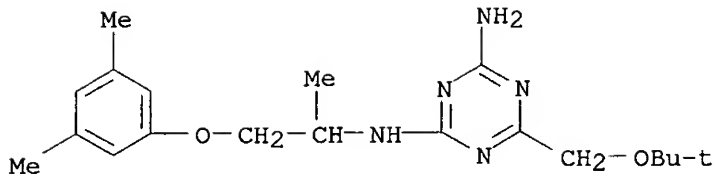


Proviso #4

L14 ANSWER 15 OF 38 CAPLUS COPYRIGHT 2002 ACS
AN 1996:628531 CAPLUS
DN 125:275917
TI Preparation of triazine derivatives as herbicides
IN Kubota, Mineyuki; Saitou, Masatoshi; Koike, Kazuyoshi; Ogawa, Shin-ichiro
PA Idemitsu Kosan Co., Ltd., Japan
SO PCT Int. Appl., 41 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9625404	A1	19960822	WO 1996-JP360	19960219
W: AL, AM, AU, BB, BG, BR, CA, CN, CZ, EE, FI, GE, HU, IS, KG, KR, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
JP 08217763	A2	19960827	JP 1995-29124	19950217
JP 3029545	B2	20000404		
CA 2213214	AA	19960822	CA 1996-2213214	19960219
AU 9646766	A1	19960904	AU 1996-46766	19960219
AU 699392	B2	19981203		
EP 810219	A1	19971203	EP 1996-902473	19960219
EP 810219	B1	20010425		
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, LU, NL				
CN 1181074	A	19980506	CN 1996-193124	19960219
AT 200779	E	20010515	AT 1996-902473	19960219
ES 2158280	T3	20010901	ES 1996-902473	19960219
US 6004902	A	19991221	US 1997-875786	19971027
PRAI JP 1995-29124	U	19950217		
WO 1996-JP360	W	19960219		

OS MARPAT 125:275917
AB The title compds. I [X1 represents linear or branched C1-4 alkyl or halogeno; n represents an integer of 0 to 4, provided that when n is an integer of 2 or above, then X1 substituents may be the same or different; and R1 represents linear or branched C1-10 alkyl optionally having one to four substituents selected from C1-4 alkoxy and/or hydroxy, provided that when the linear or branched C1-10 alkyl is substituted by two or more C1-4 alkoxy groups and/or hydroxy groups, then these substituents may be either the same or different] are prepd. The title triazine derivs. exhibit a very excellent crop/weed selectivity even under severe conditions, for example, excessively humid conditions. The title compd. II at 250 g/ha gave complete control of weeds and caused no damage to wheat.
IT **182194-62-3P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of triazine derivs. as herbicides)
RN 182194-62-3 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6-[(1,1-dimethylethoxy)methyl]-N-[2-(3,5-dimethylphenoxy)-1-methylethyl]- (9CI) (CA INDEX NAME)


Me
Me
Me
O
CH2
CH
NH
NH2
N
N
N
CH2
OBu-t

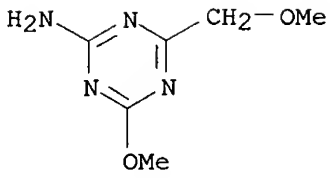
L14 ANSWER 19 OF 38 CAPLUS COPYRIGHT 2002 ACS
AN 1990:138746 CAPLUS
DN 112:138746
TI Preparation of N-arylsulfonyl-N'-arylureas via carbonylation reactions
IN Besenyei, Gabor; Nemeth, Sandor; Simandi, Laszlo; Belak, Maria; Szabo, Maria; Dukai, Jozsef; Nagy, Lajos; Tomordi, Elemer; Soptei, Csaba; Eichhardt Dioszegi, Erzsebet
PA Magyar Tudomanyos Akademia, Kozponti Kemiai Kutato Intezet, Hung.; Nitrokemia Ipartelepek
SO Ger. Offen., 17 pp.
CODEN: GWXXBX
DT Patent
LA German

same as #16.

FAN.CNT 1

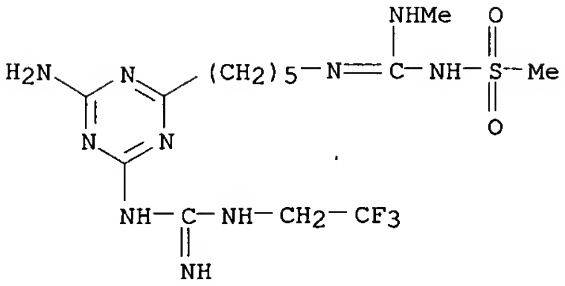
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI DE 3906910	A1	19890921	DE 1989-3906910	19890303
HU 202487	B	19910328	HU 1988-1062	19880304
AU 8930830	A1	19890907	AU 1989-30830	19890228
AU 607312	B2	19910228		
DK 8901002	A	19891002	DK 1989-1002	19890301
US 4954628	A	19900904	US 1989-317769	19890302
FR 2628106	A1	19890908	FR 1989-2771	19890303
FR 2628106	B1	19930604		
NL 8900534	A	19891002	NL 1989-534	19890303
GB 2216519	A1	19891011	GB 1989-4946	19890303
GB 2216519	B2	19911211		
ES 2010631	A6	19891116	ES 1989-1091	19890303
JP 02003664	A2	19900109	JP 1989-51808	19890303
ZA 8901642	A	19900131	ZA 1989-1642	19890303
DD 279241	A5	19900530	DD 1989-326244	19890303
PL 152515	B1	19910131	PL 1989-278104	19890303
CH 678323	A	19910830	CH 1989-797	19890303
AT 8900482	A	19930715	AT 1989-482	19890303
AT 397249	B	19940225		
CN 1038638	A	19900110	CN 1989-102524	19890304
BR 8901145	A	19891031	BR 1989-1145	19890306
PRAI HU 1988-1062		19880304		

OS MARPAT 112:138746
AB Ar1SO2NHCONHAr2 [I; Ar1 = (substituted) Ph, naphthyl, thienyl; Ar2 = (substituted) Ph, pyridyl, pyrimidinyl, triazinyl], were prepd. by 1) condensation of Ar1SO2NXY (X = Cl, Br; Y = Na, K, quaternary ammonium, phosphonium) with Ar2NH2 and CO in the presence of a carbonylation catalyst and optionally in the presence of a phase transfer catalyst, 2) condensation of Ar2NXY1 (Y1 = H, Na, K) with Ar1SO2NH2 in the presence of CO, a carbonylation catalyst, and an optional phase transfer catalyst, etc. Thus, 4-MeC6H4SO2NClNa, PdCl2, and MeCN in CH2Cl2 were pressurized to 5.0 MPa CO and the mixt. was stirred 5 h. The product mixt. was stirred 16 h with 2-amino-4-methyl-6-methoxytriazine. Solvent was removed and the residue was stirred with aq. K2CO3 to give 72.5% tosylsulfonyltriazinylurea II.,.
IT **125069-39-8**, 2-Amino-4-methoxy-6-methoxymethyltriazine
RL: RCT (Reactant)
(condensation of, with carbonylated phenylsulfonamide)
RN 125069-39-8 CAPLUS
CN 1,3,5-Triazin-2-amine, 4-methoxy-6-(methoxymethyl)- (9CI) (CA INDEX NAME)


H2N
N
CH2—OMe
N
N
OMe

CM 1

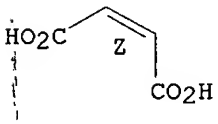
CRN 79651-58-4
CMF C14 H25 F3 N10 O2 S



CM 2

CRN 110-16-7
CMF C4 H4 O4
CDES 2:Z

Double bond geometry as shown.

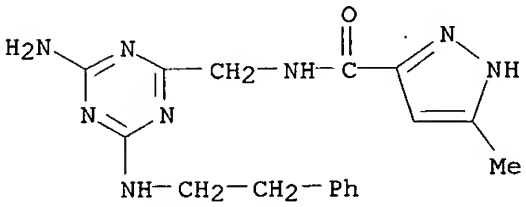


L14 ANSWER 24 OF 38 CAPLUS COPYRIGHT 2002 ACS
AN 1979:575401 CAPLUS
DN 91:175401
TI s-Triazine derivatives
IN Honna, Ryuji; Ogawa, Kazuo; Toratani, Keiko; Hashimoto, Sadao; Suzue, Takashi
PA Taiho Yakuhin Kogyo K. K., Japan
SO Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

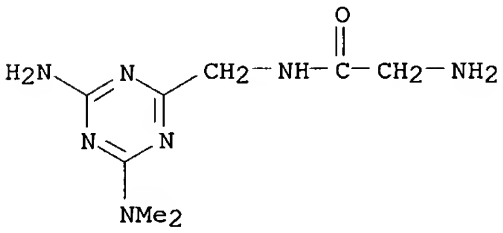
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 54044686	A2	19790409	JP 1977-109107	19770909
JP 61048516	B4	19861024		

AB Triazines I [R, R1, Z, Z1 = H, H, O, bond; Me, Me, O, bond; H, Bu, O, bond; H, PhCH2CH2, O, bond; Me, Me, NH, bond; H, Bu, NH, bond; H, H, O, CH2; H, H, O, CH:CH; H, PhCH2CH2, NH, CONHCH2; H, H, O, CONHCH2CH2] and II were prepd., e.g., by reaction of III (R2 = alkoxy) with RR1NC(:NH)NHC(:NH)NH2. Thus, a mixt. of Na, PhCH2CH2NHC(:NH)NHC(:NH)NH2.HCl, and Me 5-methyl-3-isoxazolecarboxylate in MeOH was refluxed 3 h to give 80.4% II. Hypoglycemic data of II are given in alloxan-diabetic rats.

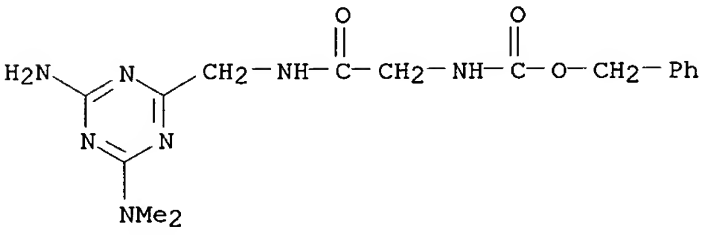
IT **71780-11-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 71780-11-5 CAPLUS
CN 1H-Pyrazole-3-carboxamide, N-[[4-amino-6-[(2-phenylethyl)amino]-1,3,5-triazin-2-yl]methyl]-5-methyl- (9CI) (CA INDEX NAME)



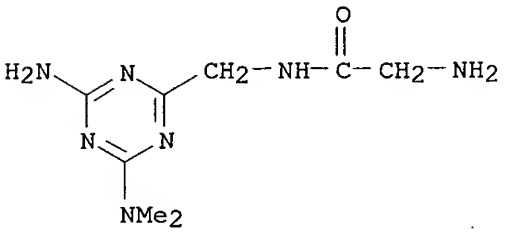
L14 ANSWER 25 OF 38 CAPLUS COPYRIGHT 2002 ACS
AN 1978:510292 CAPLUS
DN 89:110292
TI Mass spectra of triazine derivatives derived from amino acids and peptides
AU Maekawa, Kazuyuki; Taniguchi, Eiji; Kuwano, Eiichi
CS Inst. Pflanzenschutz Chem., Univ. Kyushu, Fukuoka, Japan
SO Org. Mass Spectrom. (1978), 13(1), 4-13
CODEN: ORMSBG; ISSN: 0030-493X
DT Journal
LA German
AB The mass spectra are reported of 36 triazine derivs. of amino acids and peptides which incorporate the C terminal in the triazine ring. Characteristic fragments indicating the presence of the triazine ring were obsd. which, when used as a marker, enabled estn. of the C-terminal of peptides. In dipeptides both terminals could be detd. simultaneously.
IT **40917-42-8**
RL: PRP (Properties)
(mass spectrum of)
RN 40917-42-8 CAPLUS
CN Acetamide, 2-amino-N-[[4-amino-6-(dimethylamino)-1,3,5-triazin-2-yl]methyl]- (9CI) (CA INDEX NAME)



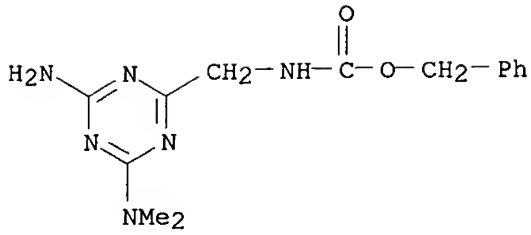
L14 ANSWER 26 OF 38 CAPLUS COPYRIGHT 2002 ACS
AN 1976:554963 CAPLUS
DN 85:154963
TI Pesticides derived from amino acids
AU Maekawa, K.; Taniguchi, E.; Kuwano, E.; Shuto, Y.
CS Fac. Agric., Kyushu Univ., Fukuoka, Japan
SO Environ. Qual. Saf., Suppl. (1975), 3(Pesticides), 748-53
CODEN: EQSSDX
DT Journal
LA English
AB Benzimidazole derivs. of amino acids and peptides contg. hydrophilic moieties, e.g., benzyloxycarbonylaminomethyl, inhibited the growth of radish seedlings and barnyard grass. 2-(1-Amino-2-phenylethyl)benzimidazole (I) [60603-62-5] (100 ppm) was active against tobacco mosaic virus. 2-[1-(Benzyloxycarbonylamino)-2-(3-indolyl)ethyl]benzimidazole [60603-49-8] and 2-[1-(benzyloxycarbonylamino)-4-guanidylbutyl]benzimidazole [60627-28-3] promoted rice seedling growth but inhibited barnyard grass. Several decarboxylated benzimidazole amino acid derivs. were also fungicidal.
IT **40917-31-5 40917-42-8 60603-74-9**
RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)
(herbicidal and pesticidal activity of)
RN 40917-31-5 CAPLUS
CN Carbamic acid, [2-[[[4-amino-6-(dimethylamino)-1,3,5-triazin-2-yl]methyl]amino]-2-oxoethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)



RN 40917-42-8 CAPLUS
CN Acetamide, 2-amino-N-[[4-amino-6-(dimethylamino)-1,3,5-triazin-2-yl]methyl]- (9CI) (CA INDEX NAME)



RN 60603-74-9 CAPLUS
CN Carbamic acid, [[4-amino-6-(dimethylamino)-1,3,5-triazin-2-yl]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)



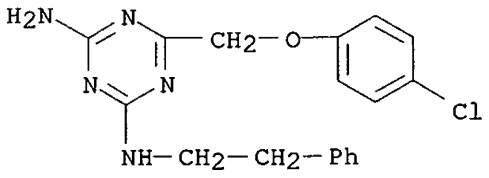
L14 ANSWER 27 OF 38 CAPLUS COPYRIGHT 2002 ACS
AN 1976:180302 CAPLUS
DN 84:180302
TI Cholesterol- and lipid-lowering 2-amino-4-(2-phenylethylamino)-6-(phenoxymethyl)-1,3,5-triazines
PA Merckle, Ludwig, K.-G., Chem.-Pharm. Fabrik, Fed. Rep. Ger.
SO Brit., 7 pp.
CODEN: BRXXAA
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	GB 1384684	A	19750219	GB 1973-59834	19731227
	DE 2263110	A1	19740711	DE 1972-2263110	19721222
	DE 2263110	B2	19800131		
	DE 2263110	C3	19800918		
PRAI	DE 1972-2263110		19721222		

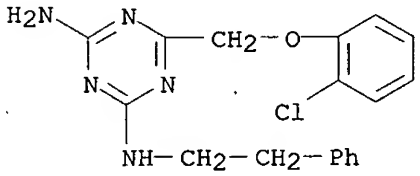
AB Nineteen title compds. I (R = H, Ac, (halophenoxy)alkanoyl; R1, R2 = H, alkyl; R3 = p-halo, o-Cl, m-CF3) were prepd. from Ph(CH2)2NHC(:NH)NHC(:NH)NH2 (II) by treatment with R3C6H4OCR1R2CO2R4 (R4 = H, Et). Thus, I (R = R1 = R2 = H, R3 = p-Cl) was prepd. (82.1%) by treating II in CHCl3 with p-ClC6H4OCH2CO2Et 6 hr at room temp. The cholesterol- and lipid-lowering activities of I were many times greater than that of Clofibrat (no data). LD50 of I were >4 g/kg and >12.5 g/kg for oral administration in rats and mice, resp.

IT **53878-49-2P 53878-55-0P 56367-09-0P**
56367-10-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(blood cholesterol and lipids lowering substance, prepn. of)

RN 53878-49-2 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6-[(4-chlorophenoxy)methyl]-N-(2-phenylethyl)-(9CI) (CA INDEX NAME)



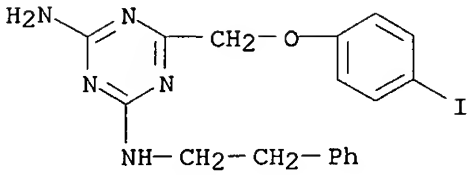
RN 53878-55-0 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6-[(2-chlorophenoxy)methyl]-N-(2-phenylethyl)-(9CI) (CA INDEX NAME)



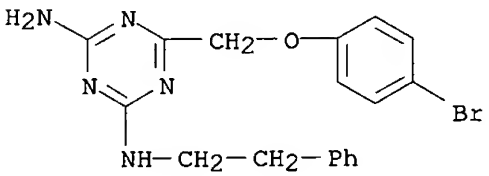
RN 56367-09-0 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6-[(4-iodophenoxy)methyl]-N-(2-phenylethyl)-

Excluded from compd claims
Previous (3)
But good for method

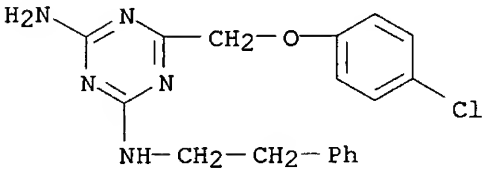
(9CI) (CA INDEX NAME)



RN 56367-10-3 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6-[(4-bromophenoxy)methyl]-N-(2-phenylethyl)-
(9CI) (CA INDEX NAME)

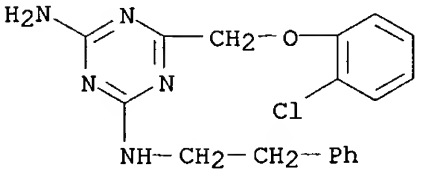


L14 ANSWER 28 OF 38 CAPLUS COPYRIGHT 2002 ACS
AN 1976:83991 CAPLUS
DN 84:83991
TI Hypolipemic activity of clofibrate-related compounds
AU Metz, G.; Specker, M.
CS Res. Dev. Dep., L. Merckle K.-G., Blaubeuren, Ger.
SO Arzneim.-Forsch. (1975), 25(11), 1686-92
CODEN: ARZNAD
DT Journal
LA English
AB Seventy clofibrate-related compds. with general structures, I, II, III, or IV, were prepd. and their hypolipemic activity was compared to that of clofibrate [637-07-0] in normal and hyperlipemic rats. Many of the compds. were as effective or more effective than clofibrate, and many of them were less toxic than clofibrate. The nature of the acid group seems to be more important for efficacy than the influence of .alpha.-methyl substitution. .alpha.-Substitution seems to be important for the differentiation of anticholesteremic and antitriglyceridemic activity.
IT **53878-49-2P 53878-55-0P 56367-09-0P**
56367-10-3P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and hypolipemic activity of)
RN 53878-49-2 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6-[(4-chlorophenoxy)methyl]-N-(2-phenylethyl)-(9CI) (CA INDEX NAME)

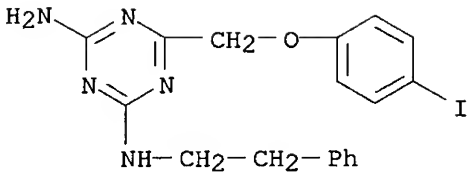


Same on 27

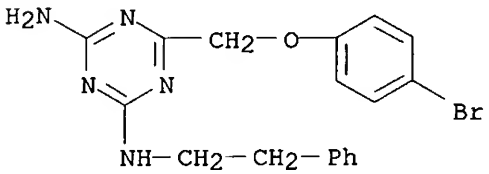
RN 53878-55-0 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6-[(2-chlorophenoxy)methyl]-N-(2-phenylethyl)-(9CI) (CA INDEX NAME)



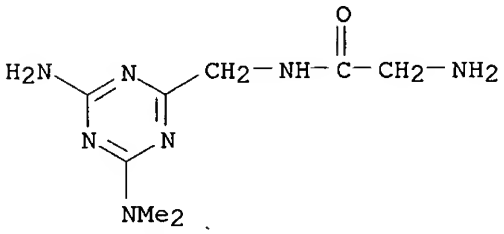
RN 56367-09-0 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6-[(4-iodophenoxy)methyl]-N-(2-phenylethyl)-(9CI) (CA INDEX NAME)



RN 56367-10-3 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6-[(4-bromophenoxy)methyl]-N-(2-phenylethyl)-(9CI) (CA INDEX NAME)



L14 ANSWER 29 OF 38 CAPLUS COPYRIGHT 2002 ACS
AN 1975:593713 CAPLUS
DN 83:193713
TI New method for the determination of peptide carboxyl groups
AU Maekawa, K.; Kuwano, E.
CS Inst. Plant Chem., Kyushu Univ., Fukuoka, Japan
SO Fresenius' Z. Anal. Chem. (1975), 276(2), 121-5
CODEN: ZACFAU
DT Journal
LA German
AB Treatment of the carboxyl groups of peptides with dimethylbiguanide gave the corresponding peptide-triazines which were hydrolyzed by Streptomyses griseus protease and the amino acid derivs. identified by thin-layer or paper chromatog.
IT **40917-42-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and enzymic hydrolysis of)
RN 40917-42-8 CAPLUS
CN Acetamide, 2-amino-N-[[4-amino-6-(dimethylamino)-1,3,5-triazin-2-yl]methyl]- (9CI) (CA INDEX NAME)



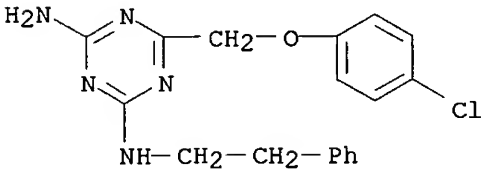
L14 ANSWER 31 OF 38 CAPLUS COPYRIGHT 2002 ACS
AN 1974:505580 CAPLUS
DN 81:105580
TI 2-Amino-4-(phenethylamino)-6-(phenoxyalkyl)-1,3,5-triazines
IN Metz, Gunter; Specker, Manfred
PA Merckle, L., K.-G., Chem.-Pharm. Fabrik
SO Ger. Offen., 13 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2263110	A1	19740711	DE 1972-2263110	19721222
	DE 2263110	B2	19800131		
	DE 2263110	C3	19800918		
	AT 7310766	A	19750615	AT 1973-10766	19731221
	AT 328459	B	19760325		
	CH 598235	A	19780428	CH 1973-18096	19731221
	GB 1384684	A	19750219	GB 1973-59834	19731227
PRAI	DE 1972-2263110		19721222		

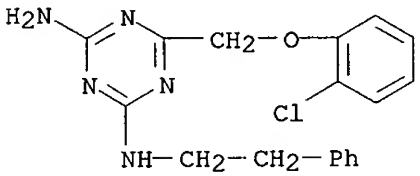
AB Seven triazines (I; Z = CH2, CH2CH2, or CHMeCH2; R = H, Ac, or COCHMeOC6H4Cl-4; R1 = Cl-2 or -4 or CF3-3), useful as anticholesteremics and antilipemics (no data), were prepd. by reaction of PhCH2CH2NHC(:NH)NHC(:NH)NH2 (II) with R1C6H4OZCO2H or their derivs., optionally followed by acylation. LD50 values of I were obtained in the rat. Thus, II reacted with 4-ClC6H4OCH2CO2Et at room temp. to give 82% I (Z = CH2, R = H, R1 = Cl-4), which was also prepd. in 47% yield by refluxing II, 4-ClC6H4OCH2CO2H, and POCl3. Re-fluxing I (Z = CH2CH2, R = H, R1 = Cl-4) and Ac2O gave 60-5% I (Z = CH2CH2, R = Ac, R1 = Cl-4).

IT **53878-49-2P 53878-55-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

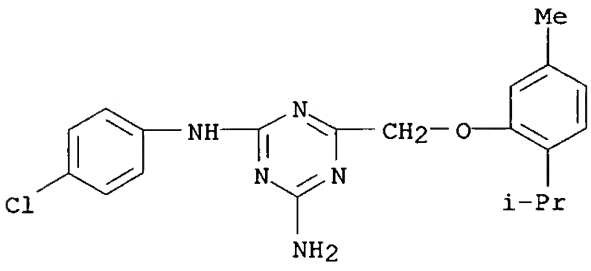
RN 53878-49-2 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6-[(4-chlorophenoxy)methyl]-N-(2-phenylethyl)-(9CI) (CA INDEX NAME)



RN 53878-55-0 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6-[(2-chlorophenoxy)methyl]-N-(2-phenylethyl)-(9CI) (CA INDEX NAME)

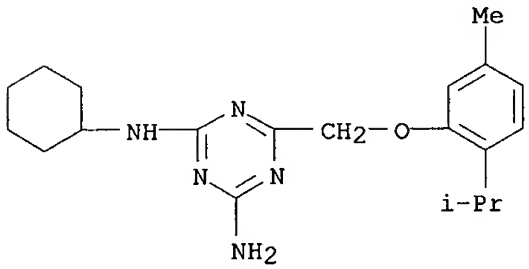


L14 ANSWER 32 OF 38 CAPLUS COPYRIGHT 2002 ACS
AN 1973:505207 CAPLUS
DN 79:105207
TI New substituted triazines and their diuretic activity
AU Guioca, Mrs. Vas.
CS Lab. Pharm. Chem., Univ. Athens, Athens, Greece
SO Ann. Pharm. Fr. (1973), 31(4), 283-92
CODEN: APFRAD
DT Journal
LA French
AB Triazines I (R = 2,3-(MeO)2C6H3CH2, p-BuC6H4CH:CH, etc.; R1 = H, R2 = Ph, cyclohexyl, Ph(CH2)2, PhCH2, p-ClC6H4; NR1R2 = piperidino, morpholino, 4-methyl-1-piperazino) (48 compds.) were prepd. in 12-77% yields by treating H2NC(:NH)NHC(:NH)NR1R2 (II) with RCO2Et. Thus, II (NR1R2 = morpholino) was heated with 2,3-(MeO)2C6H3CO2Et in presence of MeONa giving 43% I (R = 2,3-(MeO)2C6H3). I (R = 2,3-(MeO)2C6H3, 6,3-(Me2CH)MeC6H4OCH2; NR1R2 = NHC6H4Cl-p) orally had diuretic activity in rats at 10-50 mg/100 g.
IT **43075-10-1P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. and diuretic activity of)
RN 43075-10-1 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, N-(4-chlorophenyl)-6-[[5-methyl-2-(1-methylethyl)phenoxy]methyl]- (9CI) (CA INDEX NAME)

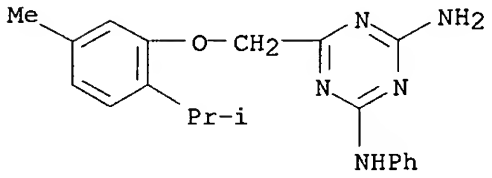


Proviso #5

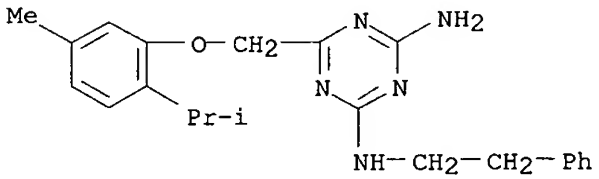
IT **43074-73-3P 43074-78-8P 43075-00-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 43074-73-3 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, N-cyclohexyl-6-[[5-methyl-2-(1-methylethyl)phenoxy]methyl]- (9CI) (CA INDEX NAME)



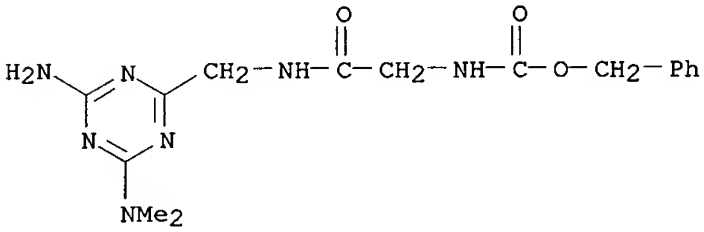
RN 43074-78-8 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6-[[5-methyl-2-(1-methylethyl)phenoxy]methyl]-N-phenyl- (9CI) (CA INDEX NAME)



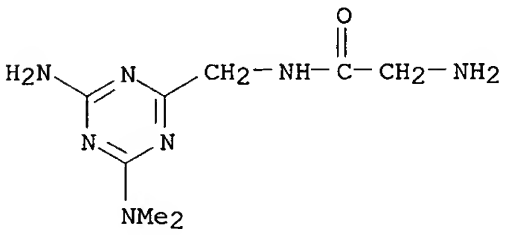
RN 43075-00-9 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6-[[5-methyl-2-(1-methylethyl)phenoxy]methyl]-N-(2-phenylethyl)- (9CI) (CA INDEX NAME)



L14 ANSWER 33 OF 38 CAPLUS COPYRIGHT 2002 ACS
AN 1973:160076 CAPLUS
DN 78:160076
TI Synthesis of 1,3,5-triazines from amino acid derivatives. III
AU Kuwano, Eiichi; Taniguchi, Eiji; Maekawa, Kazuyuki
CS Fac. Agric., Kyushu Univ., Fukuoka, Japan
SO Agr. Biol. Chem. (1973), 37(2), 423-30
CODEN: ABCHA6
DT Journal
LA German
AB Amino acid and peptide esters reacted with Me2NC(:NH)NHC(:NH)NH2 (I) to give triazines II. The Me or Et esters could be used as well as reactive esters, such as those of 1-hydroxybenzotriazole or 3-hydroxy-5-methylisoxazole. The reaction proceeded at room temp. Thus, 63% II (R = PhCH2CHNH2) was obtained by treating PhCH2CH(NH2)CO2Me with I at room temp. for 2 days. No racemization occurred. When benzyloxycarbonyl-protected dipeptides were used, the protective group could be cleaved with 25% HBr without affecting the triazine ring.
IT **40917-31-5P 40917-42-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 40917-31-5 CAPLUS
CN Carbamic acid, [2-[[[4-amino-6-(dimethylamino)-1,3,5-triazin-2-yl]methyl]amino]-2-oxoethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

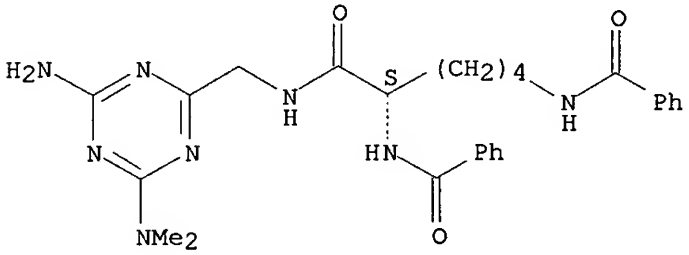


RN 40917-42-8 CAPLUS
CN Acetamide, 2-amino-N-[[4-amino-6-(dimethylamino)-1,3,5-triazin-2-yl]methyl]- (9CI) (CA INDEX NAME)

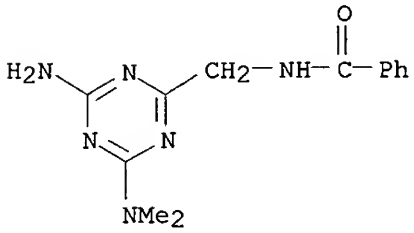


L14 ANSWER 34 OF 38 CAPLUS COPYRIGHT 2002 ACS
AN 1972:100005 CAPLUS
DN 76:100005
TI Synthesis of 1,3,5-triazines from amino acid derivatives. II
AU Kuwano, Eiichi; Taniguchi, Eiji; Maekawa, Kazuyuki
CS Fac. Agric., Kyushu Univ., Fukuoka, Japan
SO Agr. Biol. Chem. (1971), 35(11), 1759-67
CODEN: ABCHA6
DT Journal
LA German
AB The C-terminal of amino acids and peptides was modified by condensing them with biguanides in the presence of dicyclohexylcarbodiimide. The 1,3,5-triazine derivs. I [R = morpholino, R1 = Me, CH2CH2SMe, CHMe2, CH2Ph, CH2CHMe2, R2 = O2SC6H4Me-p; R = NMe2, R1 = H, Me, CH2Ph, CHMe2, CH2CH2SMe, (CH2)4NHBz, CH2CHMe2, 3-indolylmethyl, R2 = O2SC6H4Me-p, COCH2-NHO2SC6H4Me-p, Bz] were obtained in 54-5% yields.
IT **35166-15-5**
RL: PROC (Process)
(prepn. of)
RN 35166-15-5 CAPLUS
CN Benzamide, N,N'-[1-[[[[4-amino-6-(dimethylamino)-1,3,5-triazin-2-yl]methyl]amino]carbonyl]-1,5-pentanediyl]bis-, (S)- (9CI) (CA INDEX NAME)

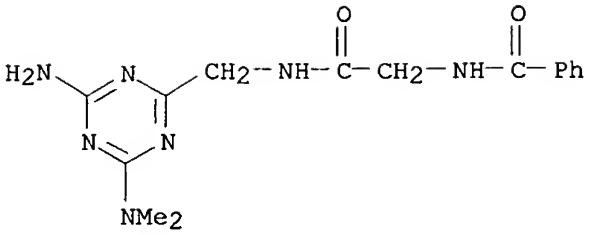
Absolute stereochemistry.



IT **35166-99-5P 35167-09-0P 35167-10-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 35166-99-5 CAPLUS
CN Benzamide, N-[[4-amino-6-(dimethylamino)-1,3,5-triazin-2-yl]methyl]- (9CI) (CA INDEX NAME)

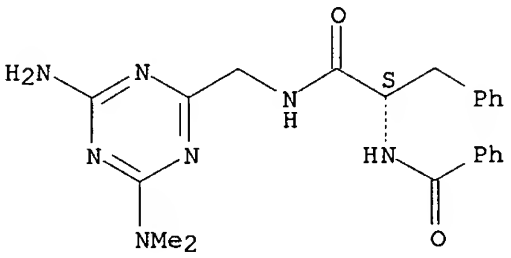


RN 35167-09-0 CAPLUS
CN Benzamide, N-[2-[[[4-amino-6-(dimethylamino)-1,3,5-triazin-2-yl]methyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

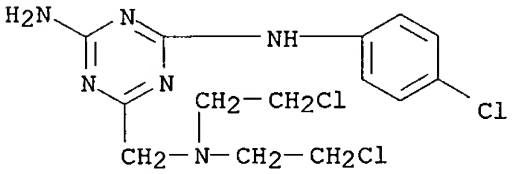


RN 35167-10-3 CAPLUS
CN Benzenepropanamide, N-[[4-amino-6-(dimethylamino)-1,3,5-triazin-2-yl]methyl]-.alpha.-(benzoylamino)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

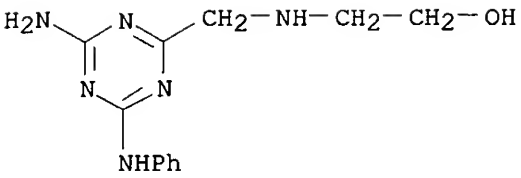


L14 ANSWER 35 OF 38 CAPLUS COPYRIGHT 2002 ACS
AN 1969:413102 CAPLUS
DN 71:13102
TI s-Triazine derivatives
AU Fel'dman, I. Kh.; Simonov, S. S.
CS Leningrad. Khim.-Farm. Inst., Leningrad, USSR
SO Khim. Geterotsikl. Soedin. (1969), (1), 154-6
CODEN: KGSSAQ
DT Journal
LA Russian
AB I (R = R1 = Cl) (5.4 g.) and 15 g. NH2C2H4OH were heated 1.5 hrs. at 100-10.degree. and cooled and 75 ml. cold H2O added to yield 5.1 g. I (R = NHC2H4OH, R1 = Cl), m. 152-4.degree. (dioxane). Similarly were obtained the following I (X = NHCH2CH2OH, Y = N(CH2CH2OH)2, Z = N(CH2CH2Cl)2, Q = NMeNH2, M = NHNHPh) (R, R1, medium, time (hrs)., temp., m.p., and % yield given): X, H, amine, 1.5, 100-10.degree., 206-8.degree. (dioxane), 71; X, OMe, amine, 1.5, 100-10.degree., 152-4.degree. (dioxane), 64; Y, H, amine, 1.5, 100-10.degree., 121-3.degree. (EtOH), 69.5; Y, Cl, BuOH, 5, reflux, 159-60.degree. (EtOH), 68.0; Y, OMe, BuOH, reflux, 159-61.degree., 66.6; Z, OMe, SOCl2, 0.5, 40.degree.-50.degree., 180.degree. (EtOH), 54; Z, Cl, SOCl2, 0.5, 40-50.degree., 183-4.degree. (EtOH), 57.5; Q, H, EtOH, 2.5, reflux, 192-4.degree. (MeOH), 57.2; Q, OMe, EtOH, 2.5, reflux, 199-201.degree. (dioxane), 54; Q, Cl, EtOH, 2.5, reflux, 200-2.degree. (dioxane), 55.4; M, H, EtOH, 2-4, 80-100.degree., 205-7.degree. (dioxane-H2O), 69.4; M, OMe, iso-PrOH, 2, water bath, 226-7.degree. (dioxane-H2O), 68.3; M, Cl, EtOH, 2-4, 80-100.degree., 218-19.degree. (BuOH), 72.1.
IT **22957-62-6P 22957-69-3P 22957-70-6P**
22957-71-7P 22957-72-8P 22957-73-9P
22957-74-0P 22957-75-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 22957-62-6 CAPLUS
CN s-Triazine, 2-amino-4-[[bis(2-chloroethyl)amino]methyl]-6-(p-chloroanilino)-, monohydrochloride (8CI) (CA INDEX NAME)

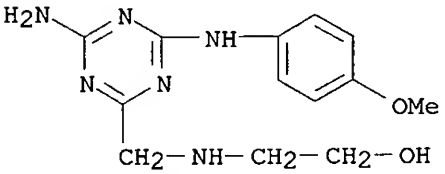


● HCl

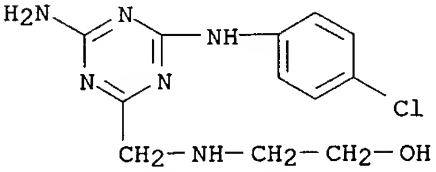
RN 22957-69-3 CAPLUS
CN Ethanol, 2-[[(4-amino-6-anilino-s-triazin-2-yl)methyl]amino]- (8CI) (CA INDEX NAME)



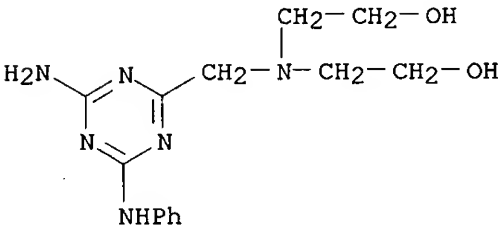
RN 22957-70-6 CAPLUS
CN Ethanol, 2-[[(4-amino-6-p-anisidino-s-triazin-2-yl)methyl]amino]- (8CI) (CA INDEX NAME)



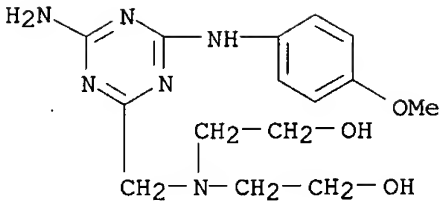
RN 22957-71-7 CAPLUS
CN Ethanol, 2-[[[4-amino-6-(p-chloroanilino)-s-triazin-2-yl]methyl]amino]- (8CI) (CA INDEX NAME)



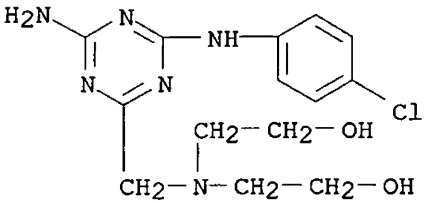
RN 22957-72-8 CAPLUS
CN Ethanol, 2,2'-[[(4-amino-6-anilino-s-triazin-2-yl)methyl]imino]di- (8CI) (CA INDEX NAME)



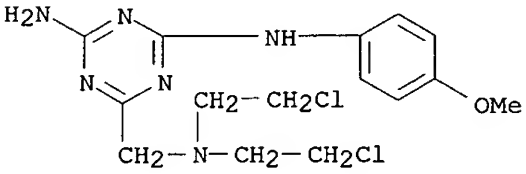
RN 22957-73-9 CAPLUS
CN Ethanol, 2,2'-[[(4-amino-6-p-anisidino-s-triazin-2-yl)methyl]imino]di- (8CI) (CA INDEX NAME)



RN 22957-74-0 CAPLUS
CN Ethanol, 2,2'-[[[4-amino-6-(p-chloroanilino)-s-triazin-2-yl]methyl]imino]di- (8CI) (CA INDEX NAME)



RN 22957-75-1 CAPLUS
CN s-Triazine, 2-amino-4-p-anisidino-6-[[bis(2-chloroethyl)amino]methyl]-, monohydrochloride (8CI) (CA INDEX NAME)



● HCl

L14 ANSWER 37 OF 38 CAPLUS COPYRIGHT 2002 ACS
AN 1967:65537 CAPLUS
DN 66:65537
TI Diamino-substituted 1,2-dihydro-1-hydroxy-1,3,5-triazines
PA Upjohn Co.
SO Brit., 22 pp.
CODEN: BRXXAA
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI GB 1053113		19661230		
PRAI US		19630419		

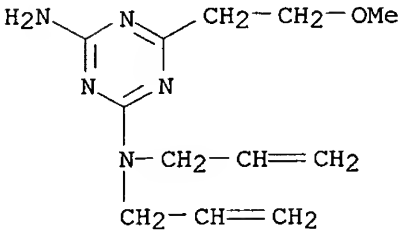
AB The title compds. (I) were prepd. by the reaction of a biguanide with a deriv. of a carboxylic acid to give a triazine (II) which is then oxidized with a perbenzoic acid to give I. Thus, a soln. of 4.6 g. Na in 100 ml. MeOH was added to 21.8 g. 1,1-diallylbiguanide-HCl in 50 ml. MeOH at 25.degree., 74. g. EtO2CH added, and the mixt. stirred 48 hrs. to give 11.6 g. II (R = H), m. 113-16.degree.. II (R = H) (5.1 g.) in 150 ml. EtOH was treated over 20 min. with 6.9 g. BzOOH in 50 ml. EtOH and the mixt. stirred 18 hrs. at 0.5.degree. to give 2.3 g. I (R = H), m. 139-41.degree.. Similarly prepd. were: II (R = Me), m. 81-2.degree.; I (R = Me), m. 132-4.degree.. Hydrogenation of I (R = Me) over PtO2 in EtOH gave the corresponding dipropylamino analog, m. 145-7.degree.. I and II similarly prepd., but using m-ClC6-H4CO2OH in the oxidn., were (R, II m.p., and I m.p. given): Et, 65-6.degree., 108.5-10.degree.; PhCH2, 58-60.degree.; oil; Bu, 32-4.degree., 82-5.degree.; cyclohexyl, 90-2.degree., 139-42.degree.; Ph, 82-4.degree., 135-45.degree.; MeOCH2CH2, - (b0.2-0.7 144-60.degree.), 132-4.degree.; Me(MeO)CHCH2, - (b0.25-0.40 145-7.degree.), - (non-cryst. oil); vinyl, 64-5.degree., - (non-cryst. oil); Pr, 50-2.degree., 88-91.degree.; iso-Pr, 49-51.degree., 119-21.degree.; n-pentyl, - (b1 155-7.degree.), - (non-cryst. oil); p-ClC6H4, 87-9.degree., 65-80.degree. (non-cryst.); PhCH2CH2, - (b0.3 180-2.degree.), 118-20.degree.; Ph(CH2)3, 57-60.degree., 91-3.degree.; cyclopropyl, 55-7.5.degree., 104-6.degree.. Similarly prepd. from 1,1-(3-oxapentamethylene)biguanide-HCl were 2-amino-4-methyl-6-morpholino-1,3,5-triazine, m. 184-5.degree., and 1,2-dihydro-1-hydroxy-2-imino-6-methyl-4-morpholino-1,3,5-triazine, m. 254-5.degree.. 2,4-Dichloro-6-methyl-1,3,5-triazine (16.4 g.) in Et2O was added over 90 min. at 0-5.degree. to 11.4 g. allylamine in Et2O to give 11.9 g. 2-allylamino-4-chloro-6-methyl-1,3,5-triazine, m. 53-6.degree.. This product was heated 2 hrs. at 100.degree. with diallylamine in Me2NCHO to give 2-allylamino-4-diallylamino-6-methyl-1,3,5-triazine, m. 40-1.5.degree., which was oxidized with m-ClC6H4-CO2OH to give 1,2-dihydro-1-hydroxy-2-allylimino-4-diallylamino-6-methyl-1,3,5-triazine, m. 78-80.degree.. Similarly prepd. were: 2-anilino-4-chloro-6-methyl-1,3,5-triazine, m. 100-15.degree.; 2-anilino-4-diallylamino-6-methyl-1,3,5-triazine, b1.1 180-95.degree.; 1,2-dihydro-1-hydroxy-4-diallylamino-6-methyl-2-phenylimino-1,3,5-triazine, m. 103-5.degree.; 2-benzylamino-4-chloro-6-methyl-1,3,5-triazine, m. 98-100.degree.; 2-benzylamino-4-diallylamino-6-methyl-1,3,5-triazine, m. 67-9.degree.; 1,2-dihydro-1-hydroxy-2-benzylimino-4-diallylamino-6-methyl-1,3,5-triazine, m. 84-6.degree.. Ir and uv spectra were given for most of the compds. prepd. The title compds. and their salts are active orally and parenterally as antihypertensives with vasodilatory activity, antisecretory agents, and central nervous system depressants. The title compds. are also intermediates in the prepn. of resins, and their salts

with fluorosilicic acid are mothproofing agents.

IT **5122-68-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 5122-68-9 CAPLUS

CN s-Triazine, 2-amino-4-(diallylamino)-6-(2-methoxyethyl)- (7CI, 8CI) (CA INDEX NAME)



L14 ANSWER 38 OF 38 CAPLUS COPYRIGHT 2002 ACS
AN 1967:65524 CAPLUS
DN 66:65524
TI 1,2-Dihydro-1-hydroxy-1,3,5-triazines
IN Ursprung, Joseph J.
PA Upjohn Co.
SO U.S., 17 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3270015		19660830	US	19630419

AB The title compds. of structure I are prepd. and are orally and parenterally active in birds and mammals, have vasodilatory activity, and are useful for lowering the blood pressure and for treatment of shock. I may be used as free base or as salts of pharmacol. accepted acids. I are prepd. by oxidn. of the proper triazine (II) with a 0-5-substituted peroxybenzoic acid (III). II are prepd. from appropriated biguanides which in turn are prepd. by treating a cyanoguanidine, NCNHC(:NH)NHR3 with a suitable R2H.HCl or by treating R2C(:NH)NHCN with R3NH2.HCl. II can also be prepd. by treating cyanuric chloride with 1 mole R1MgX to give the dichloro-s-triazine (IV) which is then treated with 1 equiv. NH3 or primary amine and with 1 equiv. secondary amine or vice versa. II may be also prepd. by treating V first with NH3 or a primary amine and then with a secondary amine. The oxidn. of II with III is carried out by mixing the reagents in an inert solvent at below 50.degree., preferably at -10 to 10.degree.. I may be isolated from the reaction mixt. by filtration, extn., or chromatography. MeONa from 4.6 g. Na in 100 ml. MeOH was added with stirring to 21.8 g. 1,1-diallylbiguanide-HCl (VI) in 50 ml. MeOH at 25.degree., 7.4 g. HCO2Et added, the mixt. stirred 48 hrs. at 25.degree. and evapd. in vacuo, and H2O added to cause the sepn. of 11.6 g. 2-amino-4-diallylamino-1,3,5-triazine (VII), m. 113-16.degree. (EtOH-H2O). BzOOH (6.9 g.) in 50 ml. EtOH was added gradually (20 min.) to 5.1 g. VII in 150 ml. EtOH at 5.degree., the mixt. stirred 18 hrs. at 0-5.degree. and evapd. in vacuo, the ppt. filtered off and washed with H2O, and the combined filtrates extd. with CHCl3 to give 1,2-dihydro-1-hydroxy-4-diallylamino-2-imino-1,3,5-triazine (VIII), m. 139-41.degree.. Addn. of 1 equiv. HCl in abs. EtOH gave the VIII.HCl salt; addn. of 2 equivs. HCl gave the VIII.2HCl salt. With EtOAc in lieu of HCO2Et the 6-Me deriv. (IX) of VII, m. 81-2.degree., was obtained. IX oxidized with BzOOH gave the 6-Me deriv. (X) of VIII, m. 132-4.degree.. Hydrogenation of X in EtOH over PtO2 at 50 lb. H and 25.degree. gave the 4-dipropylamino analog of X, m. 145-7.degree. (MeCN). VI (87 g.) in 300 ml. MeOH, MeONa (from 18.4 g. Na and 300 ml. MeOH), and 44.9 g. EtCO2Et at 25.degree. gave 57.1 g. 6-Et deriv. (XI) of VII, m. 65-6.degree. (MeOH-H2O), which (5.5 g.) oxidized in 150 ml. abs. EtOH with 9 g. m-ClC6H4CO3H (XII) at 5.degree. gave, in addn. to 1 g. unreacted XI, 2 g. 6-Et deriv. of VIII, light yellow, m. 108.5-10.degree.; it gave mono- and di-HCl and BzOH salts. Similarly 43.5 g. 1,1-(3-oxapentamethylene)biguanide-HCl, MeONa, and EtOAc gave 25.7 g. 2-amino-4-methyl-6-morpholino-1,3,5-triazine, m. 184-5.degree., which oxidized with XII gave 1,2-dihydro-1-hydroxy-2-imino-6-methyl-4-morpholino-1,3,5-triazine, m. 254-5.degree.; it formed mono- and di-HCl and mono-H3PO4 salts. Similar oxidn. of 2-amino-4-methyl-6-piperidino-1,3,5-triazine gave 1,2-dihydro-1-hydroxy-2-imino-6-methyl-4-piperidino-1,3,5-triazine. 5-Cyclohexyl-1,1-ethylenebiguanide-HCl, prepd. by fusion of ethylenimine-HCl and 3-cyclohexyl-1-cyanoguanide, reacted with EtOAc and

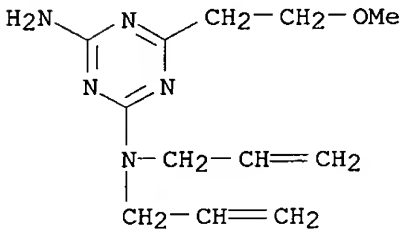
NaOMe with the formation of 2-(1-aziridinyl)-4-cyclohexylamino-6-methyl-1,3,5-triazine and oxidized with XII gave 1,2-dihydro-1-hydroxy-4-(1-aziridinyl)-2-cyclohexylimino-6-methyl-1,3,5-triazine. VI (43.5 g.) reacted with PhCH2CO2Et and NaOMe to give 28.7 g. 2-amino-4-benzyl-6-diallylamino-1,3,5-triazine, m. 58-60.degree. (MeOH-H2O), which oxidized with XII gave the 6-benzyl deriv. of VIII; it gave a pos. FeCl3 test. VI, Et valerate, and MeONa gave the 6-Bu deriv. of VII, m. 32-4.degree., which oxidized gave the 6-Bu homolog of VIII, m. 82-5.degree.. VI, Me cyclohexanecarboxylate, and MeONa gave the 6-cyclohexyl deriv. of VII, m. 90-2.degree. (MeOH-H2O) which on oxidn. gave the 6-cyclohexyl deriv. of VIII, m. 139-42.degree. (MeCN). VI (43.5 g.), 29.9 g. BzOMe, and MeONa gave the 6-Ph deriv. of VII, m. 82-4.degree. (MeOH), which oxidized gave the 6-Ph deriv. of VIII, yellow, m. 135-45.degree.. VI (65.3 g.), 30.1 g. Me acrylate, and MeONa 72 hrs. at 25.degree. gave 47 g. 2-amino-4-diallylamino-6-(2-methoxyethyl)-1,3,5-triazine, b0.2-0.7 144-60.degree., which oxidized gave light yellow 1,2-dihydro-1-hydroxy-4-diallylamino-2-imino-6-(2-methoxyethyl)-1,3,5-triazine, m. 132-4.degree. (MeCN). VI (43.5 g.), 22 g. Me crotonate, and MeONa gave the 6-(2-methoxypropyl) deriv. of VII, b0.25-0.4 145-7.degree., which oxidized gave the 6-(2-methoxypropyl) deriv. of VIII, viscous oil. VI (87 g.) was treated with MeOCH2CH2ONa (from 9.2 g. Na and 500 ml. MeOCH2CH2OH), the filtered soln. treated with 34.4 g. Me acrylate 63 hrs. at 25.degree., the concd. (in vacuo) soln. dild. with 2 l. H2O and extd. with CH2Cl2, the dried ext. fractionally distd., and the fraction, b0.45-1 138-168.degree., crystd. to give 14.9 g. 6-vinyl deriv. of VII, m. 64-5.degree. (MeOH-H2O), which oxidized with XII gave the 6-vinyl deriv. of VIII as a viscous oil. VI (43.5 g.), 22.5 g. PrCO2Me, and MeONa 69 hrs. at 25.degree. gave 33.2 g. 6-Pr deriv. of VII, m. 50-2.degree. (MeOH-H2O), which oxidized gave the 6-Pr deriv. of VIII, m. 88-91.degree. (MeCN). In the same way the 6-iso-Pr deriv. of VII, m. 49-51.degree. (EtOH-H2O), and of VIII, m. 119-21.degree., were prepd. VI and AmCO2Et gave the 6-Am deriv. of VII, b1 155-7.degree., and of VIII, yellow oil. 6-p-ClC6H4CH2 deriv. of VII, prepd. from VI and p-ClC6H4CO2Me, m. 87-9.degree., and of VIII, amorphous yellow powder, m. 65-80.degree.. VI (43.5 g.), 36.1 g. PhCH2CH2CO2Me, and MeONa 45 hrs. at 25.degree. gave 37.8 g. 6-phenenthyl deriv. of VI, viscous oil, b0.3 180-2.degree., which oxidized with XII gave the 6-phenethyl deriv. of VIII, m. 118-20.degree. (MeCN); it gave mono- and di-HCl and mono-H2SO4 salts. VI and Ph(CH2)3CO2Me gave the 6-Ph(CH2)3 deriv. of VII, yellow, m. 57-60.degree., which oxidized gave the 6-Ph(CH2)3 deriv. of VIII, m. 91-3.degree. (MeCN). VI (52.2 g.) and 26 g. Me cyclopropenecarboxylate gave the 6-cyclopropyl deriv. of VII, m. 55-7.5.degree. (EtOH-H2O), which oxidized gave the 6-cyclopropyl deriv. of VIII, m. 104-6.degree. (MeCN); its HCl, H2SO4, H3PO4, lactic, benzoic, and succinic acid salts were prepd. A soln. of 16.4 g. 2,4-dichloro-6-methyl-1,3,5-triazine (XIII) in 125 ml. Et2O was added over 1.5 hrs. to 11.4 g. allylamine in 225 ml. Et2O at 0-5.degree. and the soln. filtered and evapd. to give 11.9 g. 2-allylamino-4-chloro-6-methyl-1,3,5-triazine (XIV), m. 53-6.degree. (C6H14); it was treated with diallylamine in HCONMe, heated at 100.degree., and dild. with H2O to give 2-allylamino-4-diallylamino-6-methyl-1,3,5-triazine (XV), m. 40-1.5.degree., which oxidized with XII gave 1,2-dihydro-1-hydroxy-2-allylimino-4-diallylamino-6-methyl-1,3,5-triazine (XVI), m. 78-80.degree. (C6H14) (sintering at 72.degree.). XIII and PhNH2 gave the 2-anilino analog of XIV, m. 100-15.degree.; it reacted with diallylamine to give the 2-anilino analog of XV, yellow oil, b1.1 180-95.degree., which oxidized gave the 2-phenylimino analog of XVI, m. 103-5.degree. (C6H14). XIII and PhCH2NH2 gave the 2-benzyl-amino analog of XIV, light yellow, m. 98-100.degree. (C6H14), which was treated with diallylamine to give the

2-benzylamino analog (XVII) of XV, m. 67-9.degree.. XVII was oxidized with XII to give the 2-benzylimino analog of XVI, m. 84-6.degree. (sintering at 75.degree.) (C6H14). With these procedures 9 addnl. I and their intermediates are listed. The Me analog of X (400 mg.) in 5 ml. anhyd. Et2O was treated with 3 drops Ac2O to give 450 mg. 1,2-dihydro-1-hydroxy-2-acetylimino-4-diallylamino-6-methyl-1,3,5-triazine-AcOH, m. 91-2.degree., which with Et3N gave the free base. With AcCl in lieu of Ac2O the HCl salt was formed. With this method but using different acid anhydrides 9 addnl. I are prepd. With 18 other triazines in lieu of X 18 addnl. 1,2-dihydro-1-hydroxy-2,4-substituted-2-acetylimino-1,3,5-triazines were formed. Using 1 ml. Ac2O in 15 ml. Et2O in lieu of 3 drops and refluxing the mixt. 4 hrs. gave 1,2-dihydro-1-acetoxy-2-acetylimino-4-diallylamino-6-methyl-1,3,5-triazine. With other acid anhydrides 5 other diacylated I were prepd. The uv absorption bands of some of the compds. are given.

IT **5122-68-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 5122-68-9 CAPLUS

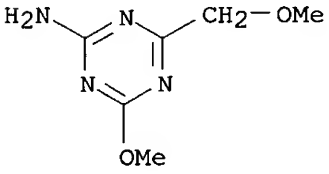
CN s-Triazine, 2-amino-4-(diallylamino)-6-(2-methoxyethyl)- (7CI, 8CI) (CA INDEX NAME)



L14 ANSWER 16 OF 38 CAPLUS COPYRIGHT 2002 ACS
AN 1996:113265 CAPLUS
DN 124:146146
TI preparation of thiazolyliminosulfonylurea derivatives as herbicides
IN Makino, Kenji; Suzuki, Hideaki; Nagaoka, Takeshi; Niki, Toshio; Hamada, Toshimasa; Kusuoka, Yoshuki; Nawamaki, Tsutomu; Watanabe, Shigeomi; Ito, Yoichi; Et, Al.
PA Nissan Chemical Ind Ltd, Japan
SO Jpn. Kokai Tokkyo Koho, 48 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 07252253	A2	19951003	JP 1995-4248	19950113
PRAI JP 1994-7703		19940127		

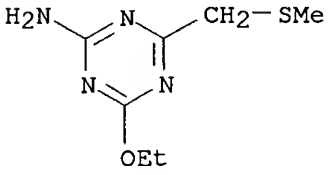
OS MARPAT 124:146146
AB The title compds. [I; R1 = alkyl, alkenyl, alkynyl, etc.; R2 = (substituted) pyrimidinyl, triazinyl, etc., bond a = satd., unsatd.] are prepd. ClSO2NCO was added dropwise to a suspension of triazine deriv. II in THF with stirring at room temp., followed by a suspension of III in THF and Et3N, and the mixt. was stirred at room temp. to give I [R1 = 3-chloroallyloxy, R2 = 4-methoxy-6-(methoxymethyl)triazin-2-yl, a = satd.], which killed >90% barnyard grass and Setaria viridis at 6.3 g/are.
IT **125069-39-8**, 2-Amino-4-methoxy-6-(methoxymethyl)triazine
RL: RCT (Reactant)
(prepn. of thiazolyliminosulfonylurea derivs. as herbicides)
RN 125069-39-8 CAPLUS
CN 1,3,5-Triazin-2-amine, 4-methoxy-6-(methoxymethyl)- (9CI) (CA INDEX NAME)



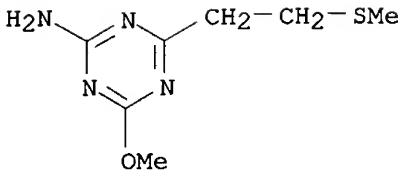
L14 ANSWER 21 OF 38 CAPLUS COPYRIGHT 2002 ACS
AN 1985:220904 CAPLUS
DN 102:220904
TI Heterocyclic substituted sulfonylureas
IN Willms, Lothar; Humburg, Gerhard; Bauer, Klaus; Bieringer, Hermann; Buerstell, Helmut
PA Hoechst A.-G. , Fed. Rep. Ger.
SO Ger. Offen., 29 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 3324800	A1	19850117	DE 1983-3324800	19830709
	EP 134477	A1	19850320	EP 1984-107831	19840705
	R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE				
	DK 8403350	A	19850110	DK 1984-3350	19840706
	DD 220217	A5	19850327	DD 1984-265012	19840706
	ES 534113	A1	19850401	ES 1984-534113	19840706
	BR 8403369	A	19850618	BR 1984-3369	19840706
	JP 60038370	A2	19850227	JP 1984-139790	19840707
	ZA 8405216	A	19850227	ZA 1984-5216	19840708
	AU 8430433	A1	19850110	AU 1984-30433	19840709
PRAI	DE 1983-3324800		19830709		

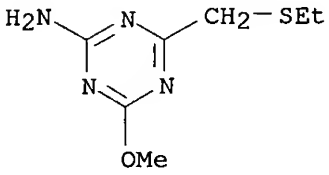
OS CASREACT 102:220904
AB Pyrimidinyl- and triazinyl(phenylsulfonyl)ureas I [R = (un)substituted Ph; R1, R2 = H, alkyl; R3 = H, alkoxy, alkylthio, CH2:CHCH2O, HC.tplbond.CHCH2O, amino, (un)substituted alkyl; R4, R5 = H, halo, (un)substituted alkyl; R6 = alkyl, alkenyl, PhCH2; X = CH2, N; n = 1-3; m = 0-2] were prepd. Thus, H2NC(:NH2)N:C(OMe)NH2.HCl in MeOH was treated with Na and MeSCH2CO2Et to give 52% 4-methoxy-6-[(methylthio)methyl]-1,3,5-triazin-2-amine. This was stirred 18 h at room temp. in CH2Cl2 with 2-ClC6H4SO2NCO to give 79.5% triazinylurea II. In preemergence tests 2.5 kg II/ha gave 80-100% control of, e.g., Stellaria media.
IT **96601-55-7 96601-56-8 96602-44-7**
RL: RCT (Reactant)
(condensation of, with benzenesulfonyl isocyanate deriv.)
RN 96601-55-7 CAPLUS
CN 1,3,5-Triazin-2-amine, 4-ethoxy-6-[(methylthio)methyl]- (9CI) (CA INDEX NAME)



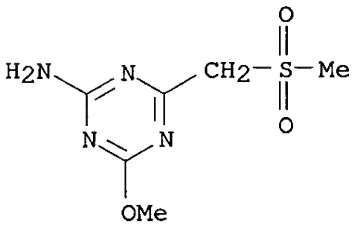
RN 96601-56-8 CAPLUS
CN 1,3,5-Triazin-2-amine, 4-methoxy-6-[2-(methylthio)ethyl]- (9CI) (CA INDEX NAME)



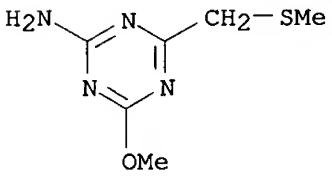
RN 96602-44-7 CAPLUS
CN 1,3,5-Triazin-2-amine, 4-[(ethylthio)methyl]-6-methoxy- (9CI) (CA INDEX NAME)



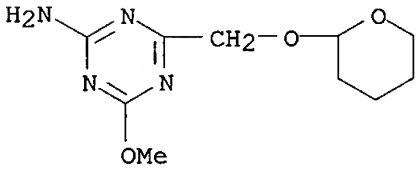
IT **96602-43-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation of, with benzenesulfonyl isocyanates)
RN 96602-43-6 CAPLUS
CN 1,3,5-Triazin-2-amine, 4-methoxy-6-[(methylsulfonyl)methyl]- (9CI) (CA INDEX NAME)



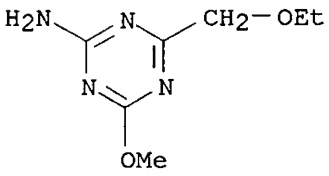
IT **96602-42-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn., oxidn., and condensation of, with benzenesulfonyl isocyanates)
RN 96602-42-5 CAPLUS
CN 1,3,5-Triazin-2-amine, 4-methoxy-6-[(methylthio)methyl]- (9CI) (CA INDEX NAME)



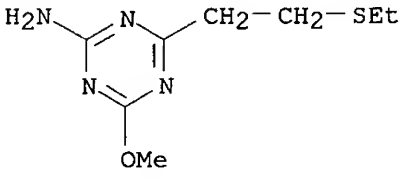
L14 ANSWER 22 OF 38 CAPLUS COPYRIGHT 2002 ACS
AN 1984:586001 CAPLUS
DN 101:186001
TI Metabolism of chlorsulfuron by tolerant broadleaves
AU Hutchison, J. M.; Shapiro, R.; Sweetser, P. B.
CS E. I. du Pont de Nemours and Co., Inc., Wilmington, DE, 19898, USA
SO Pestic. Biochem. Physiol. (1984), 22(2), 243-7
CODEN: PCBPBS; ISSN: 0048-3575
DT Journal
LA English
AB The ability of flax (Linum usitatissimum) and black nightshade (Solanum nigrum) to metabolize chlorsulfuron [64902-72-3] was studied to det. if metab. contributes to tolerance, and to identify any metabolites produced. Plant leaves were treated with [14C]chlorsulfuron for a 24-h period. The metabolites were extd., sepd. by high-performance liq. chromatog., and characterized. Mass spectral anal. and independent synthesis confirmed a major metabolite (B-1) as 2-chloro-N-[[4-(hydroxymethyl)-6-methoxy-1,3,5-triazin-2-yl]aminocarboxyl]benzenesulfonamide [87644-23-3]. A second major metabolite (B) was a carbohydrate conjugate of B-1. Plants were more tolerant to B-1 applications than to chlorsulfuron. Thus, metab. may be the basis of selectivity to chlorsulfuron for tolerant broadleaf plants as well as for grasses.
IT **92533-23-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, with chlorobenzenesulfonyl isocyanate)
RN 92533-23-8 CAPLUS
CN 1,3,5-Triazin-2-amine, 4-methoxy-6-[[(tetrahydro-2H-pyran-2-yl)oxy]methyl]- (9CI) (CA INDEX NAME)



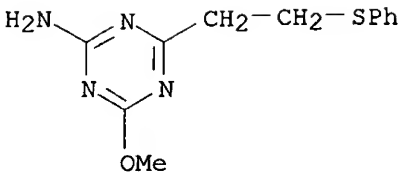
L14 ANSWER 30 OF 38 CAPLUS COPYRIGHT 2002 ACS
AN 1975:564133 CAPLUS
DN 83:164133
TI Heterocyclic compounds. I. Syntheses of 1,3,5-triazine derivatives and their pharmacological activities. 1
AU Tsujikawa, Teruaki; Takei, Saburo; Tsushima, Susumu; Tsuda, Takashi; Tsukamura, Kazuo; Sirakawa, Kenzo; Chiba, Sukehiro; Nagawa, Yuji; Yui, Tohoru
CS Cent. Res. Div., Takeda Chem. Ind., Ltd., Osaka, Japan
SO Yakugaku Zasshi (1975), 95(5), 499-511
CODEN: YKKZAJ
DT Journal
LA Japanese
AB 6-Alkoxy-2-alkyl-4-amino-1,3,5-triazines and related compds. were synthesized and their pharmacol. activities were examd. Main characteristics of these compds. after their intraperitoneal administration were divided into two categories, sedation and convulsion. The sedative effect was parallel to potentiation of barbiturate hypnosis. No clear relationship was found between anticonvulsant and sedative effects. In many cases, the compds. with phenylpiperazinyl group produced fall in blood pressure. This hypotension seems to be due at least in part, to central action of the compd.
IT **5270-22-4P 5270-25-7P 5270-28-0P**
5375-81-5P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and pharmacol. activity of)
RN 5270-22-4 CAPLUS
CN 1,3,5-Triazin-2-amine, 4-(ethoxymethyl)-6-methoxy- (9CI) (CA INDEX NAME)



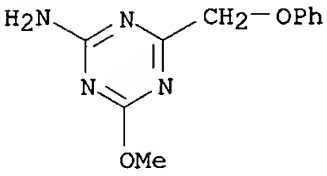
RN 5270-25-7 CAPLUS
CN 1,3,5-Triazin-2-amine, 4-[2-(ethylthio)ethyl]-6-methoxy- (9CI) (CA INDEX NAME)



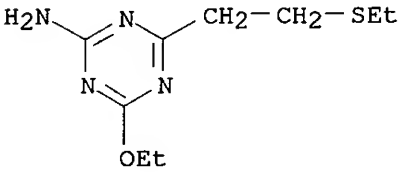
RN 5270-28-0 CAPLUS
CN 1,3,5-Triazin-2-amine, 4-methoxy-6-[2-(phenylthio)ethyl]- (9CI) (CA INDEX NAME)



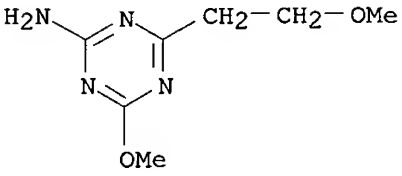
RN 5375-81-5 CAPLUS
CN 1,3,5-Triazin-2-amine, 4-methoxy-6-(phenoxymethyl)- (9CI) (CA INDEX NAME)



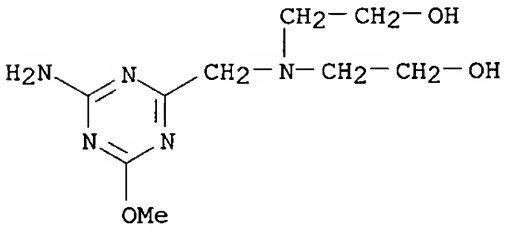
IT **56968-42-4P 56968-49-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 56968-42-4 CAPLUS
CN 1,3,5-Triazin-2-amine, 4-ethoxy-6-[2-(ethylthio)ethyl]- (9CI) (CA INDEX NAME)



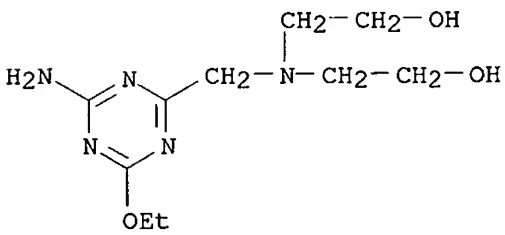
RN 56968-49-1 CAPLUS
CN 1,3,5-Triazin-2-amine, 4-methoxy-6-(2-methoxyethyl)- (9CI) (CA INDEX NAME)



L14 ANSWER 36 OF 38 CAPLUS COPYRIGHT 2002 ACS
AN 1968:459209 CAPLUS
DN 69:59209
TI Antitumor substances. VII. Reaction of N-amidino-O-alkylisourea with some carboxylic esters
AU Hayashi, Seigoro; Furukawa, Mitsuru; Yamamoto, Junko; Nishizima, Yoko
CS Fac. Pharm. Sci., Kumamoto Univ., Kumamoto, Japan
SO Chem. Pharm. Bull. (Tokyo) (1968), 16(3), 474-9
CODEN: CPBTAL
DT Journal
LA English
AB The reaction of N-amidino-O-alkylisourea with some carboxylic esters was studied. Condensation with diethyl oxalate in alc. gave alkyl 4-amino-6-alkoxy-s-triazine-2-carboxylate through formation of a five-membered-ring intermediate. Alkyl 4-amino-6-alkoxy-s-triazine-2-carboxylate was easily converted into the corresponding amide with a variety of amines. Condensation with ethyl acetoacetate gave 6-methyl-2-alkoxyamidino-4-pyrimidinol and 4-amino-2-alkoxy-6-acetomethyl-s-triazine. Condensation with ethyl cyanoacetate afforded only 4-amino-2-alkoxy-6-cyanomethyl-s-triazine, but not any expected pyrimidinol. Condensation with ethyl chloroacetate gave 4-amino-2-alkoxy-6-chloromethyl-s-triazine, which was converted into 4-amino-2-alkoxy-6-substituted amino-s-triazine with a variety of amines.
IT **19840-00-7P 19840-01-8P 19840-06-3P**
19840-07-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 19840-00-7 CAPLUS
CN Ethanol, 2,2'-[[(4-amino-6-methoxy-s-triazin-2-yl)methyl]imino]di- (8CI) (CA INDEX NAME)

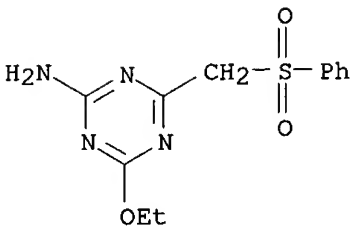


RN 19840-01-8 CAPLUS
CN Ethanol, 2,2'-[[(4-amino-6-ethoxy-s-triazin-2-yl)methyl]imino]di- (8CI) (CA INDEX NAME)

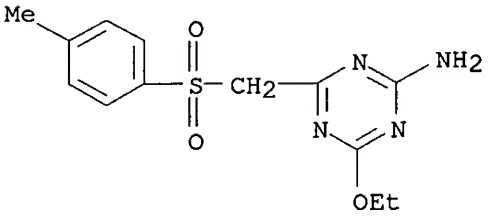


RN 19840-06-3 CAPLUS

CN s-Triazine, 2-amino-4-ethoxy-6-[(phenylsulfonyl)methyl]- (8CI) (CA INDEX NAME)



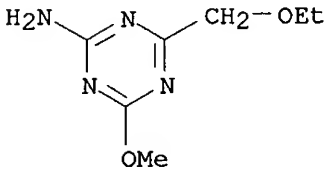
RN 19840-07-4 CAPLUS
CN s-Triazine, 2-amino-4-ethoxy-6-[(p-tolylsulfonyl)methyl]- (8CI) (CA INDEX NAME)



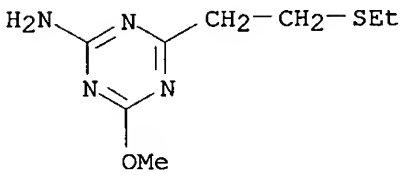
L15 ANSWER 1 OF 11 CAOLD COPYRIGHT 2002 ACS
AN CA64:12702d CAOLD
TI 2-amino-4-alkoxy-1,3,5-triazines
AU Tsuda, Takashi; Takei, S.; Tsujikawa, T.
DT Patent
TI 2-amino-4-alkoxy-S-triazines
PA Takeda Chemical Industries, Ltd.
DT Patent

PATENT NO.	KIND	DATE
JP 66001115		1966
NL 6504702		
BE 662676		
DE 1212545		
FR 1432109		
GB 1030587		

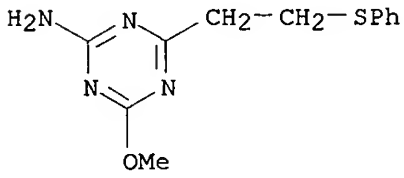
IT **5270-22-4** **5270-25-7** **5270-28-0**
5375-81-5
RN 5270-22-4 CAOLD
CN 1,3,5-Triazin-2-amine, 4-(ethoxymethyl)-6-methoxy- (9CI) (CA INDEX NAME)



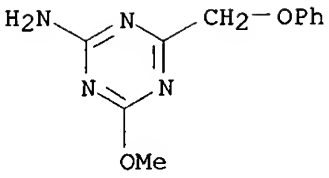
RN 5270-25-7 CAOLD
CN 1,3,5-Triazin-2-amine, 4-[2-(ethylthio)ethyl]-6-methoxy- (9CI) (CA INDEX NAME)



RN 5270-28-0 CAOLD
CN 1,3,5-Triazin-2-amine, 4-methoxy-6-[2-(phenylthio)ethyl]- (9CI) (CA INDEX NAME)



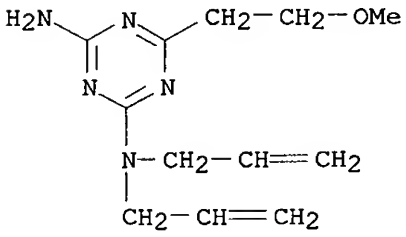
RN 5375-81-5 CAOLD
CN 1,3,5-Triazin-2-amine, 4-methoxy-6-(phenoxymethyl)- (9CI) (CA INDEX NAME)


H2N
N
CH2—OPh
N
N
OMe

L15 ANSWER 2 OF 11 CAOLD COPYRIGHT 2002 ACS
AN CA64:5117f CAOLD
TI 1,2-dihydro-2-imino-1,3,5-triazine 1-ether derivs.
PA Upjohn Co.
DT Patent

PATENT NO.	KIND	DATE
NL 6501753		
US 3270018		1966

IT **5122-68-9**
RN 5122-68-9 CAOLD
CN s-Triazine, 2-amino-4-(diallylamino)-6-(2-methoxyethyl)- (7CI, 8CI) (CA INDEX NAME)



L31 ANSWER 1 OF 8 MARPAT COPYRIGHT 2002 ACS
AN 136:263168 MARPAT
TI Preparation of substituted heterocyclic aryl-alkyl-aryl compounds as thrombin inhibitors
IN Isaacs, Richard C.; Williams, Peter D.; Lyle, Terry A.; Staas, Donnette D.; Savage, Kelly L.
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 91 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

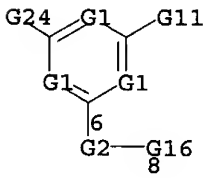
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2002022584	A1	20020321	WO 2001-US28791	20010911

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI US 2000-231656P 20000911

AB Title compds. I [u, v, w = CH, N; X = 0, SO0-2, NH, alkenyl, C:O, C:ONH, C:OO, alkyl, CH2NH, CH2O, CF2; Y = (CH2)0-1(CR4R5)(CH2)0-1; Z = O, S0-2, C:O, amino, CF2, bond; R1 = H, alkyl(CN), C:O, (CH2)0-1-carboxy, CF3, alkoxy, halo, SO0-2, amino; R2 = (un)substituted Ph, 5-6-membered heterocycle; R3 = Ph, (un)substituted ring system, 5-6-membered heterocycle; R4-5 = H, alkyl; R6, R8 = halo, alkylamino, heterocycle] were prepd. Examples include data for over 20 compds., 3 solid oral dosage formulations and an in-vitro assay for protease detn. for example compds. For instance, 2'-isopropyl-5-methylbiphenyl-3-ol (prepd. in 3 steps from 2-isopropylphenyl iodide) was reacted with (S)-2-(pyridin-4-ylamino)propan-1-ol to give II isolated as the trifluoroacetate. Example compds. exhibited inhibitory activity against human thrombin, Ki < 24 nM. I are useful in the treatment of blood coagulation and cardiovascular disorders.

MSTR 1



G1 = N
G5 = CH2
G6 = O
G14 = S
G15 = alkyl<(1-4)>
G24 = Hy<EC (1-2) Q (0-) N (0-) O (0-) S (0) OTHERQ, AR (0), BD (ALL) SE, RC (1), RS (1) E6> (SO (1-3) alkyl<(1-8)>)
G29 = CH2

MPL: claim 1
NTE: substitution is restricted
NTE: or pharmaceutically acceptable salts

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

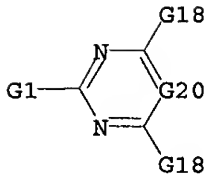
L31 ANSWER 2 OF 8 MARPAT COPYRIGHT 2002 ACS
AN 135:33374 MARPAT
TI Nitrosulfobenzamides, processes for their preparation, and their use in the production of sulfonylurea herbicides
IN Ford, Mark James; Vermehren, Jan
PA Aventis Cropscience G.m.b.H., Germany
SO PCT Int. Appl., 59 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2001042226	A1	20010614	WO 2000-EP11501	20001118
W: AE, AG, AL, AM, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CN, CR, CU, CZ, DM, DZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KP, KR, KZ, LC, LK, LR, LT, LV, MA, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TT, UA, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2001020092	A1	20010906	US 2000-732006	20001207

PRAI DE 1999-19959291 19991209

AB The invention relates to nitrosulfobenzamides I [wherein R1, R2 = (un)substituted C1-10 (preferably C1-6) hydrocarbon radical; or NR1R2 = (un)substituted 3- to 8-membered heterocyclic ring optionally contg. 1 or 2 further N/O/S ring heteroatoms; Q = H or cation]. I can be used advantageously for the prepn. of sulfonylurea herbicides, and their precursors such as sulfonyl chlorides or sulfonamides. For instance, reaction of 4-nitro-2-sulfobenzoic acid dipotassium salt with phosgene in PhMe in the presence of DMF and pyridine, followed by removal of excess phosgene and then addn. of dimethylamine, gave title compd. I [R1 = R2 = Me, Q = K] in 90% yield and 80% purity (isolated). Alternatively, prepn. and further treatment of the above product in situ with phosgene and then with ammonia gave N,N-dimethyl-2-aminosulfonyl-4-nitrobenzamide in 81% yield and 93.4% purity. When this sulfonamide intermediate was treated yet again with phosgene and then with 2-amino-4,6-dimethoxypyrimidine, the sulfonylurea deriv. II [X = NO2] was obtained in 58% yield and 87% purity. Hydrogenation of the latter in formic acid in the presence of Na molybdate gave II [X = NHCHO], i.e. foramsulfuron, in 83.6% yield and 95.5% purity. Foramsulfuron was also prepd. using I via another invention route with earlier introduction of the formamide moiety.

MSTR 5



G1 = NH2
G4 = S
G5 = alkyl<(1-6)> (SO (1-) G19)
G18 = alkyl<(1-6)> (SO (1-) G19)
G19 = alkoxy<(1-4)>
G20 = N
MPL: claim 18

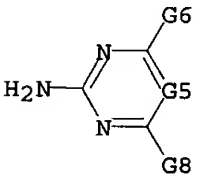
RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 3 OF 8 MARPAT COPYRIGHT 2002 ACS
AN 130:95383 MARPAT
TI Preparation of aryne intermediates useful in herbicide manufg.
IN Harrington, Philip M.; Kremer, Kenneth A. M.
PA American Cyanamid Company, USA
SO U.S., 9 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5856576	A	19990105	US 1998-15817	19980129
	CN 1187485	A	19980715	CN 1998-103947	19980106
PRAI	US 1998-15817		19980129		

OS CASREACT 130:95383
AB The title compds. [I; R = H, CN, F, etc.; X = NO2, NR1R2; Z = OH, Br, Cl, OSO2R3; R1, R2 = H, CHO, Ac, etc.; R3 = C1-6 alkyl, C1-6 haloalkyl, (un)substituted Ph], useful intermediates in the manuf. of herbicidal compds., were prepd. by palladium catalyzed coupling of an o-halonitrobenzene or o-haloaniline with 3-butyne-1-ol.

MSTR 8



G3 = alkoxy<(1-3)>
G5 = N
G6 = alkylthio<(1-4)> (SO (1-) G3)
G8 = alkyl<(1-4)> (SO (1-) G3)
MPL: claim 17

RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

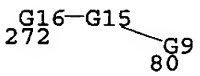
L31 ANSWER 4 OF 8 MARPAT COPYRIGHT 2002 ACS
AN 129:275833 MARPAT
TI Combinatorial synthesis and screening of .alpha.-ketoamide-derivative cysteine protease inhibitors
IN Blandino, Carmen M.; Coffen, David L.; Chipman, Stewart D.; Cheng, Hong
PA Arqule, Inc., USA
SO PCT Int. Appl., 71 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9846559	A1	19981022	WO 1998-US7747	19980416
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9871290	A1	19981111	AU 1998-71290	19980416
EP 975584	A1	20000202	EP 1998-918344	19980416
R: CH, DE, DK, FR, GB, IT, LI, NL, SE				

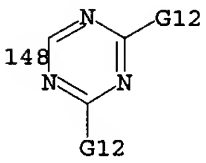
PRAI US 1997-843584 19970416
WO 1998-US7747 19980416

AB Via combinatorial synthesis, about 38,000 .alpha.-ketoamide derivs. were prepd. and the arrays screened, from which 6 compds. were isolated which had a high inhibitory activity against three cysteine proteases: cruzain, papain, and cathepsin B; these title compds. may be useful in the treatment of diseases (e.g., Chagas' disease) assocd. with these proteases. Thus, Me 2-(2-benzothienyl)-2-oxoethanoate was amidated with 4-aminobenzyl amine, the intermediate isolated and reacted with benzyl isothiocyanate, producing ther 2-benzothienyl .alpha.-ketoamide I which demonstrated an IC50 for cruzain of 2.2 .mu.M and 3.3 .mu.M for cathepsin B.

MSTR 2



G2 = NH
G9 = 148



G10 = S
G12 = alkyl (SO (1-) G3)
G17 = alkyl (SO (1-) G3)
G18 = O
G19 = acyl
MPL: claim 17
NTE: also incorporates claim 53

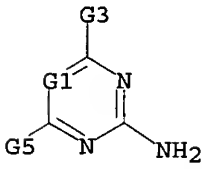
L31 ANSWER 5 OF 8 MARPAT COPYRIGHT 2002 ACS
AN 127:262707 MARPAT
TI Substituted aryl sulfonyl(thio)ureas used as herbicides
IN Gesing, Ernst Rudolf F.; Kirsten, Rolf; Kluth, Joachim; Muller, Klaus-Helmut; Drewes, Mark Wilhelm; Jansen, Johannes Rudolf; Philipp, Ulrich; Riebel, Hans-Jochem; Schallner, Otto; Dollinger, Markus; Santel, Hans-Joachim
PA Bayer A.-G., Germany; Gesing, Ernst Rudolf F.; Kirsten, Rolf; Kluth, Joachim; Muller, Klaus-Helmut; Drewes, Mark Wilhelm; Jansen, Johannes Rudolf; Philipp, Ulrich; Riebel, Hans-Jochem; et al.
SO PCT Int. Appl., 54 pp.
CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9732861	A1	19970912	WO 1997-EP798	19970220
	W: AU, BB, BG, BR, BY, CA, CN, CZ, HU, IL, JP, KR, KZ, LK, MX, NO, NZ, PL, RO, RU, SK, TR, UA, US				
	RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	DE 19608445	A1	19970911	DE 1996-19608445	19960305
	CA 2248068	AA	19970912	CA 1997-2248068	19970220
	AU 9720917	A1	19970922	AU 1997-20917	19970220
	AU 712363	B2	19991104		
	EP 885200	A1	19981223	EP 1997-906098	19970220
	R: DE, DK, ES, FR, GB, IT				
	CN 1212686	A	19990331	CN 1997-192820	19970220
	BR 9707917	A	19990727	BR 1997-7917	19970220
PRAI	DE 1996-19608445	19960305			
	WO 1997-EP798	19970220			

AB The invention relates to novel substituted arylsulfonyl(thio)ureas I and their salts [wherein A = N or CH; Q = O or S; R1 = H, halo, or (un)substituted alkyl, alkoxy, alkylthio, alkylamino, dialkylamino, cycloalkyl, cycloalkyloxy, or heterocyclyloxy; R2 = H, halo, or (un)substituted alkyl, alkoxy, alkylthio, alkylamino, dialkylamino, cycloalkyl, cycloalkyloxy, or heterocyclyloxy; R3 = H or (un)substituted alkyl; R4 = (un)substituted alkyl, alkoxy, alkenyl, alkynyl, alkenyloxy, alkynyloxy, cycloalkyl, cycloalkyloxy, or cycloalkylalkyl; and R5 = H, formyl, or (un)substituted alkyl, alkylcarbonyl, alkoxycarbonyl, alkylsulfonyl, alkenyl, alkynyl, cycloalkyl, cycloalkylcarbonyl, cycloalkylsulfonyl, or heterocyclyl; except for the compd. N-(4,6-dimethylpyrimidin-2-yl)-N'-[[2-(1,1,2,2-tetrafluoroethoxy)-6-methylphenyl]sulfonyl]urea]. Also disclosed are a process for producing the novel compds., and their use as herbicides. For example, condensation of 2-methoxy-6-methylbenzenesulfonamide with 2-[N,N-bis(phenoxycarbonyl)amino]-4,6-dimethoxy-1,3,5-triazine in MeCN in the presence of KOBu-tert, followed by stirring with 1N aq. HCl and CH2Cl2, gave 55% title compd. II. At 30 g/ha preemergence, II gave complete kill of 6 test plants: Alopecurus, Lolium, Sorghum, Amaranthus, Chenopodium,

and Stellaria.

MSTR 2



G1 = N
G3 = alkylthio (SO (1-) G11)
G5 = alkyl (SO (1-) G11)
G11 = alkoxy<(1-4)>
MPL: claim 4

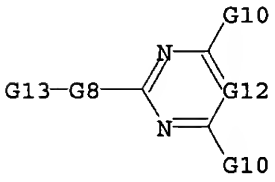
L31 ANSWER 6 OF 8 MARPAT COPYRIGHT 2002 ACS
AN 124:146187 MARPAT
TI Preparation of N-[acylamino(carbamoyl)phenylsulfonyl]-N'-pyrimidinylureas as herbicides and plant growth regulators
IN Schnabel, Gerhard; Willms, Lothar; Bauer, Klaus; Bieringer, Hermann
PA Hoechst Schering Agrevo GmbH, Germany
SO Ger. Offen., 27 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 4415049	A1	19951102	DE 1994-4415049	19940429
	CA 2189044	AA	19951109	CA 1995-2189044	19950412
	WO 9529899	A1	19951109	WO 1995-EP1344	19950412
	W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TT, UA, UZ, VN				
	RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	AU 9523441	A1	19951129	AU 1995-23441	19950412
	EP 757679	A1	19970212	EP 1995-917311	19950412
	EP 757679	B1	19981021		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL				
	CN 1147252	A	19970409	CN 1995-192788	19950412
	CN 1066140	B	20010523		
	HU 76144	A2	19970728	HU 1996-2966	19950412
	BR 9507562	A	19970805	BR 1995-7562	19950412
	JP 09512538	T2	19971216	JP 1995-527953	19950412
	AT 172456	E	19981115	AT 1995-917311	19950412
	ES 2125012	T3	19990216	ES 1995-917311	19950412
	RO 114894	B3	19990830	RO 1996-1949	19950412
	ZA 9503436	A	19960117	ZA 1995-3436	19950428
	US 5922646	A	19990713	US 1997-906238	19970804
	CN 1295067	A	20010516	CN 2000-108955	20000524
PRAI	DE 1994-4415049	19940429			
	WO 1995-EP1344	19950412			

US 1995-429933 19950427

AB Title compds. [I; R = halo, alkyl, alkoxy; R1 = H, (un)substituted hydrocarbyl(oxy); R2 = H, (un)substituted hydrocarbyl; NR1R2 = heterocyclyl; R3 = acyl; R4 = H, aliph. hydrocarbyl; W1,W2 = O, S; X,Y = halo, alkyl, alkoxy, etc.; Z = CH or N; n = 0-3] were prepd. as herbicides and plant growth regulators (no data). Thus, 2,4-(H2N)(O2N)C6H3CO2H was converted in 7 steps 2-dimethylaminocarbonyl-5-methoxycarbonylaminobenzenesulfonamide which was condensed with 4,6-dimethoxy-2-(phenoxycarbonylamino)pyrimidine to give title compd. II.

MSTR 3



G8 = NH
G10 = alkyl<(1-6)> (SO (1-) G11) / alkylthio<(1-6)> (SO (1-) G11)
G11 = alkoxy<(1-4)>
G12 = N
MPL: claim 5

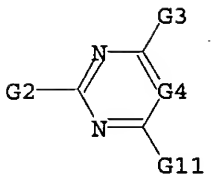
L31 ANSWER 7 OF 8 MARPAT COPYRIGHT 2002 ACS
AN 121:9426 MARPAT
TI Preparation of thienylsulfonylureidoazine herbicides.
IN Gesing, Ernst R. F.; Santel, Hans Joachim; Luerssen, Klaus; Schmidt, Robert Rudolf
PA Bayer A.-G., Germany
SO Ger. Offen., 15 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI DE 4232417	A1	19940331	DE 1992-4232417	19920928
EP 590416	A1	19940406	EP 1993-114858	19930915
R: BE, CH, DE, FR, GB, IT, LI, NL				
US 5430006	A	19950704	US 1993-124919	19930921
JP 06199848	A2	19940719	JP 1993-257547	19930922
US 5508441	A	19960416	US 1995-412432	19950329

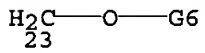
PRAI DE 1992-4232417 19920928
US 1993-124919 19930921

AB Title compds. [I; R1 = Et, Pr; R2 = H, Me; X, Y = H, OH, amino, cyano, halo, alkyl, cycloalkyl, haloalkyl, alkoxyalkyl, alkoxy, haloalkoxy, alkoxyalkoxy, alkylthio, alkylamino, dialkylamino; Z = N, CH, CR3; R3 = halo], were prepd. as herbicides (no data). Thus, Ph chloroformate was added to a mixt. of 2-ethoxycarbonylthiophene-3-sulfonamide and Et3N in MeCN; after 30 min. methanesulfonic acid and 2-amino-4-methoxy-6-methyl-s-triazine were added followed by 30 min. reflux to give title compd. II. Several I were said to show very strong herbicidal activity and good compatibility with crop plants.

MSTR 5



G2 = NH2
G3 = 23



G4 = N
G6 = Me
G11 = alkylthio<(1-4)>
MPL: claim 4

L31 ANSWER 8 OF 8 MARPAT COPYRIGHT 2002 ACS
AN 115:183348 MARPAT
TI Preparation of (pyridylsulfonyl)ureas as herbicides and plant growth regulators
IN Kehne, Heinz; Willms, Lothar; Ort, Oswald; Bauer, Klaus; Bieringer, Hermann
PA Hoechst A.-G., Fed. Rep. Ger.
SO PCT Int. Appl., 74 pp.
CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 5

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9110660	A1	19910725	WO 1990-EP2308	19901224
	W: AT, AU, BB, BG, BR, CA, CH, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MC, MG, MW, NL, NO, RO, SD, SE, SU, US				
	RW: AT, BE, BF, BJ, CF, CG, CH, CM, DE, DK, ES, FR, GA, GB, GR, IT, LU, ML, MR, NL, SE, SN, TD, TG				
	DE 4000503	A1	19910711	DE 1990-4000503	19900110
	AU 9170484	A1	19910805	AU 1991-70484	19901224
	AU 648058	B2	19940414		
	EP 510032	A1	19921028	EP 1991-901751	19901224
	EP 510032	B1	19961113		
	R: BE, CH, DE, ES, FR, GB, GR, IT, LI, NL				
	BR 9007976	A	19921110	BR 1990-7976	19901224
	HU 61746	A2	19930301	HU 1992-2275	19901224
	JP 05503514	T2	19930610	JP 1991-502068	19901224
	US 5635451	A	19970603	US 1992-859513	19920608
	US 5494886	A	19960227	US 1994-337139	19941110
PRAI	DE 1990-4000503	19900110			
	DE 1990-4030577	19900927			
	DE 1990-4030557	19900927			
	WO 1990-EP2308	19901224			

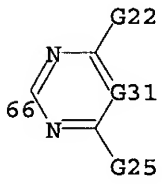
US 1992-859513 19920608
US 1993-108896 19930818

AB The title compds. [I; R = SO2NHC(:W)NR3A; A = (un)substituted pyrimidinyl, triazinyl, etc.; R1 = iodo, NR6R7, OSO2NR4R5; R2 = H, (halo)alkyl, halo, NO2, cyano, etc.; R3 = H, Me; R4 = H, alkyl, alkenyl, alkynyl, alkoxy; R5 = H, alkyl, alkenyl, alkynyl; R4R5 = (CH2)4-5, CH2CH2OCH2CH2; R6 = H, (halo)alkenyl, (un)substituted alkyl, alkylsulfonyl, PhSO2, etc.; R7 = (un)substituted alkylsulfonyl, PhSO2; R6R7 = (CH2)mSO2; W = O, S; m = 3, 4; n = 0, 1] were prepd. Thus, PhCH2SH was condensed with 2-fluoro-3-iodopyridine and the product converted in 2 steps to I (R = SO2NHR10, R1 = iodo, R2 = H) (II; R10 = H) which was condensed with R12NHCO2Ph (R12 = pyrimidinyl group Q) to give II (R10 = CONHQ). The latter gave complete control of 6 weeds, e.g., Avena sativa, at 0.3 kg/ha preemergent.

MSTR 5

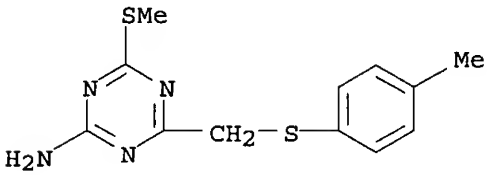
H---G7---G21

G7 = NH
G21 = 66



G23 = alkylene<(1-3)>
G24 = alkoxy<(1-3)>
G25 = alkylthio<(1-3)> (SO (1-) G26)
G31 = N
DER: or salts
MPL: claim 5

L36 ANSWER 1 OF 5 CHEMCATS COPYRIGHT 2002 ACS
Accession No. (AN): 1998:635165 CHEMCATS
Catalog Name (CO): Maybridge HTS
Publication Date (PD): 6 Feb 2002
Order Number (ON): SPB 06116
Chemical Name (CN): 4-[[(4-methylphenyl)thio]methyl]-6-(methylthio)-1,3,5-triazin-2-amine
CAS Registry No. (RN): **265314-66-7**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :

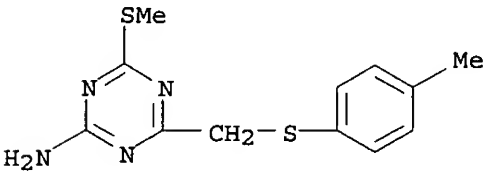


=> d l36 REF

L36 ANSWER 1 OF 5 CHEMCATS COPYRIGHT 2002 ACS
Accession No. (AN): 1998:635165 CHEMCATS

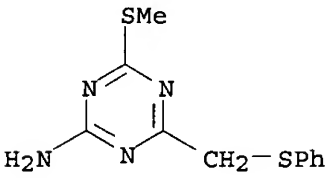
=> d l36 1-5

L36 ANSWER 1 OF 5 CHEMCATS COPYRIGHT 2002 ACS
Accession No. (AN): 1998:635165 CHEMCATS
Catalog Name (CO): Maybridge HTS
Publication Date (PD): 6 Feb 2002
Order Number (ON): SPB 06116
Chemical Name (CN): 4-[[(4-methylphenyl)thio]methyl]-6-(methylthio)-1,3,5-triazin-2-amine
CAS Registry No. (RN): **265314-66-7**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :

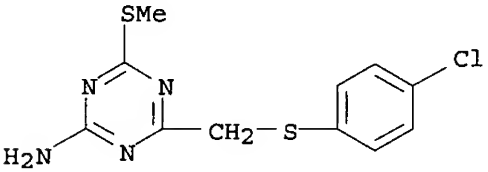


L36 ANSWER 2 OF 5 CHEMCATS COPYRIGHT 2002 ACS
Accession No. (AN): 1998:635164 CHEMCATS
Catalog Name (CO): Maybridge HTS
Publication Date (PD): 6 Feb 2002
Order Number (ON): SPB 06115

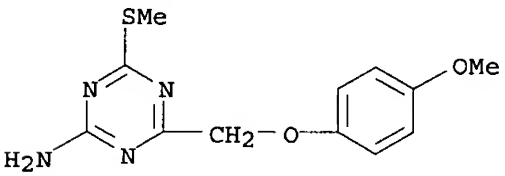
Chemical Name (CN): 4-(methylthio)-6-[(phenylthio)methyl]-1,3,5-triazin-2-amine
CAS Registry No. (RN): **265314-65-6**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



L36 ANSWER 3 OF 5 CHEMCATS COPYRIGHT 2002 ACS
Accession No. (AN): 1998:635163 CHEMCATS
Catalog Name (CO): Maybridge HTS
Publication Date (PD): 6 Feb 2002
Order Number (ON): SPB 06114
Chemical Name (CN): 4-[[(4-chlorophenyl)thio]methyl]-6-(methylthio)-1,3,5-triazin-2-amine
CAS Registry No. (RN): **265314-64-5**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



L36 ANSWER 4 OF 5 CHEMCATS COPYRIGHT 2002 ACS
Accession No. (AN): 1998:634797 CHEMCATS
Catalog Name (CO): Maybridge HTS
Publication Date (PD): 6 Feb 2002
Order Number (ON): SPB 05667
Chemical Name (CN): 4-[(4-methoxyphenoxy)methyl]-6-(methylthio)-1,3,5-triazin-2-amine
CAS Registry No. (RN): **266679-33-8**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



L36 ANSWER 5 OF 5 CHEMCATS COPYRIGHT 2002 ACS

Accession No. (AN): 1998:634796 CHEMCATS
Catalog Name (CO): Maybridge HTS
Publication Date (PD): 6 Feb 2002
Order Number (ON): SPB 05666
Chemical Name (CN): 4-[(2-chlorophenoxy)methyl]-6-(methylthio)-1,3,5-triazin-2-amine
CAS Registry No. (RN): **266679-32-7**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :